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IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re Application of: Jonathan S. Brecher)
U.S. Serial No.: To Be Assigned)
Filed: Herewith (February 11, 2000))
(This application claims the benefit of U.S.)
Provisional Application Serial No. 60/119,930)
Filed on February 12, 1999))
Title: DERIVING CHEMICAL STRUCTURAL)
INFORMATION)

Box Patent Application
Assistant Commissioner for Patents
Washington, D.C. 20231

TRANSMITTAL LETTER

Dear Sir:

Enclosed herewith for filing in the above-referenced application are the following documents:

1. New U.S. Patent Application entitled **DERIVING CHEMICAL STRUCTURAL INFORMATION**
and naming as inventor(s): Jonathan S. Brecher
the Application including 50 pages comprising:
33 pages of specification including
2 pages of claims (claims 1-4) and;
1 page of abstract; and
17 pages of informal drawings (Figures 1 to 7G).
2. Declaration and Power of Attorney (unexecuted).
3. Appendix: NOMTOKENS and Cover Sheet for Appendix:NOMTOKENS.
4. Microfiche Appendix (382 frames on 4 sheets of microfiche).

PATENT
Attorney Docket No. 103544.127

5. Postcard.

The Commissioner is hereby **not authorized** to charge the filing fees to our Deposit Account No. 08-0219.

Respectfully submitted,

HALE AND DORR LLP

Dated: February 11, 2000

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DERIVING CHEMICAL STRUCTURAL INFORMATION

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims the benefit of United States Provisional
5 Application Serial No. 60/119,930 entitled DERIVING A CHEMICAL
STRUCTURE FROM A CHEMICAL NAME filed on February 12, 1999,
incorporated herein.

REFERENCE TO MICROFICHE APPENDIX

A microfiche appendix forms part of this application. The appendix,
10 which includes a source code listing relating to an embodiment of the invention,
includes 382 frames on 4 sheets of microfiche.

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objection to the facsimile reproduction by anyone of the patent document as it
15 appears in the Patent and Trademark Office file or records, but otherwise
reserves all copyright rights whatsoever.

Background of the Invention

This application relates to deriving chemical structural information.

A chemical substance is commonly represented in textual form ("name")
20 or graphical form ("structure"), each of which has its own advantages. For
example, a name such as "benzene" is well-suited for use in a conversational or

written statement such as "The object was immersed in 100% benzene." Benzene can also be represented by a structure (Fig. 1) that illustrates that a benzene molecule features high symmetry, including six carbon atoms arranged at the corners of a regular hexagon, with six hydrogen atoms arranged a fixed distance outward from respective corners.

A chemical substance can have multiple chemical names. For example, benzene is also known as "benzol", "cyclohexatriene", "1,2,3-cyclohexatriene", "cyclohexa-1,2,3-triene", "[6]annulene", and "1-carbapyridine". Some names are sanctioned by at least one of three major organizations that have developed chemical nomenclature systems: the International Union of Pure and Applied Chemistry ("IUPAC"), the International Union of Biochemistry and Molecular Biology ("IUBMB"), and the Chemical Abstracts Service ("CAS"), a division of the American Chemical Society ("ACS"). These organizations often disagree about the preferred name for a substance, and the recommendations from each organization tend to be complex and have changed over time. In many instances, chemists produce or use chemically correct names that vary from the "sanctioned" names. Unintentional errors such as typographical errors are common.

Chemical names are commonly found in one of two general forms, known as "normal" (e.g., "O-acetylsalicylic acid") and "inverted" (e.g., "salicylic acid, O-acetyl-"). Each form has its utility. The normal form corresponds to

regular English writing style, is read from left to right, and is appropriate for use in prose. The inverted form emphasizes the main chemical feature of the substance and is particularly well suited for indexing, since the inverted form allows substances of similar chemistry to be sorted together, alphabetically.

5 Many chemical names are available only in inverted form.

The abundance of different names for the same chemical substance can create confusion and uncertainty when one chemist attempts to understand a written document produced by another chemist. Chemical structures, on the other hand, tend to cause less confusion and uncertainty.

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Summary of the Invention

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A method and a system are provided for deriving, from chemical names, corresponding structures with high accuracy and comprehensiveness. An implementation in a high speed computer allows chemical names to be accurately converted to chemical structures in real time or nearly in real time, which provides users with a powerful, practical tool for use in situations where structural representations offer substantial advantages. In at least some cases, the method and the system are able to derive such structures where the names do not conform to any sanctioned nomenclature system. By grouping chemical name fragments into a small number of classifications, the method and the system feature flexibility that facilitates application of the method and the system

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to new chemical names as well as old chemical names, including names for organic and inorganic substances. The method and the system handle inverted names, including inverted names with missing commas or with extraneous spaces.

5 Other features and advantages will become apparent from the following description, including the drawings, and from the claims.

Brief Description of the Drawings

Fig. 1 is an illustration of a chemical structure.

Fig. 2 is a block diagram of computer-based systems.

10 Figs. 3A-3B and 4 are flow diagrams of computer-based procedures.

Figs. 5A-5D, and 6 are illustrations of computer data.

Figs. 7A-7G are illustrations of output produced by software.

Detailed Description

This application is filed simultaneously with a United States Patent

15 Application entitled ENHANCING STRUCTURE DIAGRAM GENERATION,

serial no. _____, which is incorporated herein.

Fig. 2 illustrates a structure derivation system 10. A chemical name 12 is supplied via one or more input systems such as end-user keyboard input 14, file-based input 16, or World-Wide Web query input 18. The chemical name is received by computer-based internal processing 20, which derives structural output in one or more forms such as a diagram 22 displayed on paper or on a

screen, a chemical format file 24, or a graphical format file 26. One or more of the output forms may be derived from another of the output forms, e.g., by scanning a paper printout into a computer file, or by using a graphic display program to display or print a diagram based on the contents of a format file.

5 In general, in a preferred embodiment, the internal processing operates by comparing portions of the chemical name to text strings that have been predetermined to have respective characteristics and properties in accordance with rules of chemical nomenclature, and with exceptions to such rules, and assembling a structure from pieces corresponding to selected text strings, as described below.

10 Figs. 3A-3B illustrate a method 100 of the internal processing, which is applied in a specific example ("Phenacyl bromide, p-napthoxy") after the following description. The chemical name ("original input name") is preprocessed to standardize its formatting and to simplify subsequent operations
15 (step 1010). In an initial stage of the preprocessing, the individual characters of the name are manipulated as follows without reference to the chemical meaning implied by the characters. The name is converted to all lower-case characters. Common typographical errors, including errors that relate to inadvertent addition, deletion, or transposition of characters, are identified using substring
20 searches and are corrected. Uncommon characters of chemical significance are

spelled out using common characters, so that, for example, the character “μ” (“μ”) is changed to “mu”.

Also during the preprocessing, if the name or a portion of the name has been submitted in inverted form (e.g., “acetic acid, 2-hydroxy-”), the name or portion is converted to its uninverted form (e.g., “2-hydroxyacetic acid”) by a procedure 2000 (Fig. 4). A chemical name is uninverted by identifying name fragment boundaries and reordering the name fragments in accordance with a normal form. Commas are common delimiters of such name fragments, but other delimiters are found as well, and not all commas serve as boundaries. In the identification, false boundaries are determined from context and are discarded.

In the uninversion process, fragments are reordered after all fragments are identified, and context is observed. An inverted name of the form a/b/c/d/e may or may not uninvert to e/d/c/b/a; the name may become e/b/a/c/d or any of several other possibilities. The contents of each fragment are examined to determine the fragment's proper position relative to preceding fragments.

The uninversion process includes the following steps (Fig. 4). The input name is analyzed to mark all potential name fragment boundaries (step 2010). In a specific embodiment, the mark used is an @ sign, which is rarely used in chemical names. In another embodiment, it may be advantageous to use a non-printing character such as control-A (ASCII value 1) that has effectively no chemical significance.

The name is scanned from left to right and is copied, possibly with changes as now described, into a new temporary buffer (step 2020). During scanning, open- and close-parentheses and other enclosing marks are counted, and depths of enclosing marks are monitored. With some exceptions, characters
5 are copied to the new buffer unmodified. Commas that are not enclosed within any level of enclosing marks are not copied, but are instead converted to @ signs. For simplicity, any space characters or additional commas immediately following such a comma are treated as having no syntactic significance, and are not copied.

Hyphens are also examined during the scan. If a hyphen is immediately followed by a space character and is not immediately preceded by a comma or a plus ("+") or slash ("/") character, the hyphen is converted to an @ sign. Any space characters or additional commas immediately following such a hyphen are treated as having no syntactic significance, and are ignored. Such treatment addresses a common typographical error of omitting a comma, such as the
10 comma that should be present before the final word in "benzoic acid, 2-chloro- oxime".

An apostrophe that immediately precedes a digit is also assumed to represent the typographical omission of a comma, and is treated as if a comma were present. Thus, a comma is inserted between the two pertinent characters,
15 unless the characters are not enclosed in any levels of enclosing marks such as parentheses, in which case an @ sign is inserted instead.

From this point, actions occur within the temporary buffer (step 2030) and do not change the length of the buffer, which has the same length as the name in the buffer.

The buffer is scanned for the presence of a text string ("substring") "+@-",
5 which, if found, is replaced by a substring "+,-".

The buffer is scanned for the presence of a substring "mer" followed by
any character except "c". Since such a sequence, if present, indicates with high
likelihood the presence of a polymer descriptor such as a monomer, dimer, or
oligomer descriptor in the remainder of the string, any @ signs present in the
remainder of the string, i.e., to the right of the "mer" substring, are converted to
spaces. Determining whether the "mer" substring is followed by the character "c"
is important to avoid misinterpreting mercury compounds as polymers, so that,
for example, "acetic acid@mercury (ii)@hydrate" is not erroneously converted to
"acetic acid@mercury (ii) hydrate".

15 The buffer is scanned for any single one of the characters "0", "1", "2", "3",
"4", "5", "6", "7", "8", "9", "?", or an apostrophe, that is immediately followed by
any number (i.e., including zero) of the characters "]", ")", "}", or "h", in any order,
but that is not preceded by the character "d". If such a sequence is found, any @
sign that immediately follows the sequence is converted to a comma, so that, for
20 example, "1h@3h@5h@2@4@6-pyrimidinetrione" is properly converted to
"1h,3h,5h,2,4,6-pyrimidinetrione".

If the final character of the buffer is a hyphen, and the last @ sign, if present, in the buffer is preceded immediately by a single one of the characters "]", ")", or "}", which is in turn preceded by any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", or an apostrophe, the last @ sign is
5 converted to a comma.

The buffer is scanned for any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", or an apostrophe, followed immediately by a close parenthesis, followed immediately by any number of the characters "]", ")", or "}", followed immediately by an @ sign, followed immediately by any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", or "?". If such a sequence is
10 found, the @ sign is converted to a comma.

The buffer is scanned for an @ sign immediately preceding any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "a", "b", "A", or "B". If such an @ sign is found where that preceding character is preceded by either of
15 the characters "a" or "b", which is preceded by any of the characters "(", "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?" or a comma or an apostrophe, the @ sign is converted to a comma. Accordingly, for example, "4aa@8ab-dihydronaphthalene" is properly converted to "4aa,8ab-dihydronaphthalene".

The buffer is scanned for an @ sign immediately preceding any single one
20 of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", or an apostrophe, where character precedes any single one of the characters ")", "]", "]", "e", "z", "r",

"s", "E", "Z", "R", or "S". If such an @ sign is found that is preceded by any single one of the characters "e", "z", "E", or "Z", which is preceded by any of the characters "(", "[", "{", "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?" or a comma or an apostrophe, the @ sign is converted to a comma.

5 The buffer is scanned for an @ sign immediately preceding any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "a", "b", "A", "B", or an apostrophe, where such character itself precedes any single one of the characters "e", "z", "r", "s", "E", "Z", "R", or "S", or a period. If such an @ sign is found that is preceded by any number of the characters ")", "]", "}", or "*", which is preceded by any one of the characters "r", "s", "R", or "S", which is preceded by any of the characters "(", "[", "{", "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "a", "b", "A", "B", "?" or a comma or an apostrophe, the @ sign is converted to a comma.

The buffer is scanned for any occurrences of the strings "@ar@" or ",ar@". Any such string that is found is converted to ",ar,".

15 The buffer is scanned for an @ sign immediately preceding any number of periods, where such periods (if any) themselves precede either i) any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "n", "o", "p", "s", "N", "O", "P", or "S"; or ii) any of the text strings "cis", "trans", "alpha", "beta", "gamma", "delta", or "epsilon". If such an @ sign is found that is preceded by any number 20 of apostrophes or periods, which are preceded by any one of the strings "alpha", "beta", "gamma", "delta", "cis", or "trans", the @ sign is converted to a comma.

The buffer is scanned for an @ sign immediately preceding any number of periods, where such periods (if any) precede either i) any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "n", "o", "p", "s", "N", "O", "P", or "S"; or ii) any of the text strings "ortho", "meta", or "para". If such an @ sign is found that is preceded by any number of apostrophes or periods, which are preceded by any one of the strings "ortho", "meta", or "para", the @ sign is converted to a comma.

The buffer is scanned for an @ sign immediately preceding any number of periods, where such periods (if any) precede either i) any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "n", "o", "p", "s", "N", "O", "P", or "S"; or ii) any of the text strings "cis", "trans", "alpha", "beta", "gamma", "delta", or "epsilon". If such an @ sign is found that is preceded by any number of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", or an apostrophe, which are preceded by any single one of the characters "n", "o", "p", "s", "N", "O", "P", or "S", which is preceded by either i) no characters at all or ii) any single one of the characters "(", "[", "{", "-", an apostrophe, a comma, or a space, the @ sign is converted to a comma.

The foregoing regarding buffer scanning is also described by the following text strings formatted in accordance with regular expression notation, as described in Friedl, Jeffrey E. and Oram, Andy, eds., Mastering Regular Expressions, O'Reilly & Associates, 1997.

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s/+@-/+,-/gi
s/(@.*mer[^c].*)@/$1,/gi
s/([^\d][0-9\?\v][\]\h]*)@/$1,/gi
s/([0-9\?\v])@([^\@]*-$)/$1,$2/gi
s/([0-9\?\v]\v)[\]\v]@([0-9\?])/$1,$2/gi
5 s/([\v, 0-9\?\v][ab])@([0-9\?ab])/$1,$2/gi
s/([0-9,\(\v[ez])@([0-9\?\v]*[ezrs\v])/$1,$2/gi
s/([0-9ab,\(\v[rs]\v*\v])@([0-9ab\?\v]*[rsez\v])/$1,$2/gi
s/[@,]ar@/,ar,/gi
s/(alpha | beta | gamma | delta | cis | trans)[\.\.]*\.( [nops0-9\?]| cis | trans | alpha | beta | gamma | de
lta | epsilon) /$1,$2/gi
10 s/(ortho | meta | para)[\.\.]*\.( [nops0-9\?]| ortho | meta | para) /$1,$2/gi
s/([[@, \-\([][nops] [0-9\?]*\.( [nops0-9\?]| alpha | beta | gamma | delta | epsilon) /$1,$2/gi

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All remaining @ signs are treated as true name fragment boundaries, so that the buffer is broken into fragments at the @ signs and is reassembled as follows (step 2040) in an output buffer created to store a final string.

The first fragment is added to the output buffer. Each name fragment subsequent to the first fragment is treated sequentially in one of the three following ways.

- (1) A name fragment that terminates in a hyphen is prepended to the contents of the output buffer.
20 - (2) A name fragment that does not end with one of the strings in Table 1 (Fig. 5A), that does not start with one of the strings in Table 2 (Fig. 5B), that does

not contain any of the strings in Table 3 (Fig. 5C), and that does not contain the string “mer” followed by a character other than “c”, is prepended to the output buffer. The instant name fragment, when prepended, is separated from the rest of the buffer by a space character if the instant name fragment is the overall
5 second fragment to be identified and if the first fragment was one of the strings listed in Table 4 (Fig. 5D); otherwise the instant name fragment is separated from the rest of the buffer by a hyphen. (It is to be understood that Tables 1-4 are not necessarily exhaustive, and may be adapted as necessary.)

10 (3) In all other cases a name fragment is appended to the output buffer with a space character therebetween.

At this point, the uninversion process is complete and makes available the final contents of the output buffer to serve as the uninverted name (step 2050). Preprocessing is complete.

Once preprocessed, the name is divided into a series of fragments (Figs. 15 3A-3B, step 1020). In particular, the name is divided into the smallest number of meaningful fragments of a maximum length. For example, “pentane” is not divided into three fragments “penta”, “n”, and “e”, since the latter two fragments would not be meaningful, but rather is divided into two meaningful fragments “pent” and “ane”. In a specific embodiment, a fragment is determined to be 20 meaningful (“recognized”) if an exact match for the fragment is found in a dictionary of known text strings (“lexicon”) that is maintained by the system.

Each known text string is associated in the lexicon with at least one data object known as a nomToken (Fig. 6). A nomToken includes the text of the known text string as its name and is described by Type and Subtype data members, which allow similar fragments to be grouped in accordance with two levels of similarity. Examples of NomTokens are identified in this application's Appendix: NomTokens which is submitted herewith and is incorporated herein, and in which NomTokens are provided in the following format:

name{ | synonym | synonym | ... }<space>type<space>subtype<space>data

(It is to be understood that the Appendix: NomTokens is not necessarily exhaustive, and may be amended as necessary.)

A text string may be present more than once in the lexicon if the text string is associated with multiple different nomTokens. For example, the text string "amide" is associated with a first nomToken of type kTypeAcid to be used with a name such as "propanamide" and is also associated with a second nomToken, of type kTypeAcidPart2, to be used with a name such as "propanic acid amide". Each nomToken also contains a repeat count and an indicator that indicates whether a repeat count of 1 originated explicitly with the designator "mono", and other optional type-specific information. In a specific embodiment, some of the fields of the nomToken are completed within the lexicon, and others are populated through further processing.

Four data objects within a nomToken record the nomToken's chemical

significance: a connection table, a locant map, an attach-in map, and an attach-out map. The connection table includes information that specifies which atoms are connected to which bonds and information regarding characteristics such as atom types, charges, and isotopy. The locant map associates names of

5 individual atoms with respective specific locations in the connection table. For example, an atom named "2" in "2-hydroxy-propanoic acid" may be a specific one of the carbon atoms, and a "3" atom may be a different one of the carbon atoms.

Multiple locants can refer to the same atom: "beta" may refer to the same atom as did "2" above.

10 The attach-in map functions similarly to the locant map and stores a list of atoms identified in the connection table that are considered to be awaiting attachment. Such a list is particularly useful when constructing structures of esters of acids. The attach-out map associates a specific bond order to an attachment. For example, after the phrase "oct-3-ylidene" is interpreted, an entry 15 in the attach-out map indicates that the "3" atom in the "oct" group should have an attachment of order 2. For both the attach-in and attach-out maps, the actual construction of the attachments is performed later in the process.

An attach-in indicates an atom that, in at least some circumstances, preferentially has another fragment attached to it. For example, "acetate" has 20 four atoms: two carbons and two oxygens. A proper interpretation of "methyl acetate" specifies that the methyl group is attached to a particular one of the

oxygens. For a portion of the processing period, between the time that "acetate" is handled and the time that "methyl" is attached to it, an attach-in exists on that particular one of the oxygens. Then, when it is time to add the "methyl" fragment, the position indicated by the attach-in is where the "methyl" fragment is attached to the acetate.

In an example involving an attach-out, a fragment "prop" is acquired, indicating a chain of three carbon atoms. There are two ways the fragment can be attached to another fragment: (1) connecting from the first carbon atom, which would cause the three carbons to extend from the other fragment much as a flag extends from a flagpole to flap in the wind, and (2) connecting from the second carbon atom, which produces in a Y-like structure. (Connecting from the third carbon atom is, in most cases, equivalent to connecting from the first carbon atom.) One way that an attach-out may be added to a structure is via the fragment "yl". When interpreting the fragment "propyl", an attach-out is created at the default atom, which is the first carbon atom in this particular case. A name such as "propylbenzene" is consistent with the three carbon atoms of the "propyl" group sticking out in a row from the benzene fragment. On the other hand, the positioning of the attach-out may be specified explicitly. For the fragment "prop-2-yl", the attach-out is attached to the central carbon atom. A name such as "prop-2-ylbenzene" specifies that the three carbon atoms from the "prop" group are attached to the benzene in the Y-like pattern.

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A locant is a name for a specific atom. In the "prop-2-ylbenzene" example above, "2" is a name for the second atom in the "prop" three-carbon chain. In this particular case, the name happens to be neatly descriptive since "2" is used for the second atom, but such a situation cannot be assumed. Each atom may have zero locants, one locant, or multiple locants. For example, "prop-beta-yl" would be the same as "prop-2-yl"; the central atom actually has three locants that can be used interchangeably: "2", "b", and "beta". Additionally, the set of locants for a given nomToken may change (i.e., one or more may be added, and one or more may be removed as no longer valid) during the course of processing.

As the preprocessed name is parsed into fragments, a parallel list is derived from the nomTokens corresponding to each fragment (step 1030). If a fragment is represented by more than one nomToken, the nomToken having the highest-ranked type is chosen, at least initially. Punctuation characters including spaces and commas are interpreted as delimiting adjacent fragments, but are not preserved. Unrecognized fragments are converted into nomTokens of type kTypeUnknown and are included in the given order relative to the recognized nomTokens. The parallel list also stores, for each nomToken, an identification of the type of character that immediately preceded the fragment in the preprocessed name: an open parenthesis, bracket, brace, or the start of the name; a space character; or another type of character.

The recognition of parentheses and other enclosing marks, if any, is

integral to the name fragmentation process. During the fragmentation, the phrase surrounded by the innermost pair of enclosing marks is parsed as a unit, and is then consolidated as a unit according to a consolidation process described below with respect to the full name. Accordingly, each group within a set of enclosing marks is treated as a single unit, which is consistent with the syntactic meaning of enclosing marks. All levels of enclosing marks are handled in the same way, recursively.

When complete, the list of nomTokens is examined sequentially to determine whether any series of $2 \dots n$ adjacent nomToken names could be concatenated into a larger "buildable" nomToken (step 1040). This is due at least in part to the fact that a small number of chemical terms are commonly expressed with included punctuation, which the fragmentation process uses to divide the input name. For example, the phrase "mg/ml" could be interpreted as possibly unrecognized nomTokens "mg" and "ml". Accordingly, "mgml" is recognized as a nomToken of type kTypeBuildable, which allows the two nomTokens "mg" and "ml" to be combined into one nomToken. The resulting nomToken of type kTypeBuildable is then converted to a nomToken of identical name and next-highest rank. For example, a fragment "xxxx" may be associated with three nomTokens, all named "xxxx", with respective values of 73, 42, and 21. The fragment may start off with the nomToken of value 73 and then may be converted to the "next-highest rank" nomToken, of value 42, and may

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subsequently be converted to the next "next-highest rank" nomToken, of value

21.

The list of nomTokens is searched for a nomToken of type kTypeStopword, examples of which are identified in the Appendix: NomTokens
5 (step 1050). If such a nomToken is found, the found nomToken and all subsequent nomTokens are removed from the list and are discarded (step 1060).

This is due at least in part to the fact that chemical names are commonly found
with additional descriptive text immediately following (e.g., "acetic acid"
followed by "99% solution"), where the descriptive text does not contribute any
information regarding the chemical structure of the chemical substance. The
descriptive text is recognized and removed so that the remainder (e.g., "acetic
acid") can be analyzed effectively.
10

At the conclusion of the fragmentation process, the text string of the
original input name has been successfully divided into one or more substrings,
15 and a list of nomTokens has been constructed corresponding to a list of the
substrings. The fragmentation process has focused primarily on information
contained in the text itself (e.g., the sequence of characters and punctuation), not
on the chemical significance of the resulting nomTokens.

A consolidation process derives, from a list of nomTokens, a smaller list
20 that contains fewer nomTokens, e.g., one nomToken (step 1070). The
consolidation process examines the environments of the nomTokens, i.e., the

types and subtypes of each nomToken and other nearby nomTokens, and then, in each case, joins two or more nomTokens into a single replacement nomToken, as described below.

The consolidation process may determine that one or more nomTokens
5 are misidentified. For example, a nomToken of type kTypeNatDeriver serves only to modify another nomToken that refers to a natural product, i.e., a nomToken of type kTypeRoot and subtype kSubtypeNatural. NomTokens of kTypeRoot pertain to collections of atoms connected by collections of bonds in a predetermined pattern, and correspond roughly to "root" or "core" fragments of a molecule.
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In the absence of a nomToken that refers to a natural product, the nomToken of type kTypeNatDeriver is determined to have been misidentified. In such a case, the nomToken of type kTypeNatDeriver is converted to an identically-named nomToken of next-highest-rank, if any. If no identically-named nomToken of lower rank is found, the nomToken is converted to a nomToken of type kTypeUnknown, which is the lowest possible rank.
15

One suitable system of ranking of types is described herein (see also Appendix: NomTokens and the source code appendix under "enum nomTokenType"), but there are other suitable systems of ranking as well. With 20 any suitable system of ranking, all consolidation steps are to be considered in light of the characteristics of that system of ranking. In at least some cases, it is

important that nomTokens be considered and acted upon in a particular order, so that nomTokens of the necessary rank are available when needed, and have not already been examined and converted to other nomTokens of lower rank.

The consolidation process begins with environments that are most specific. For example, characteristically, nomTokens of type kTypeCrown are immediately preceded and immediately followed by numerals, which are represented by nomTokens of type kTypeUnknown, for fragments consisting entirely of numeric digits. If such environments are found, a connection table for a crown ether may be constructed, and all three nomTokens may be replaced by a single nomToken containing the connection table. A nomToken of type kTypeCrown that is not preceded and followed by numerals is determined to be misidentified and is, as described above, therefore converted into the next-highest-ranked nomToken and retained in the list for later processing.

Consolidation continues with a series of less-localized nomenclature types characterized as sometimes appearing in multiple non-adjacent fragments. For example, interpretation of atomic chains may be performed at this stage. A nomToken of type kTypePrefix, such as "pent" or "penta", may refer implicitly to an alkyl or heteroatomic chain. The "penta" in "pentadiene" necessarily refers to a five-carbon chain. In a suitable environment, when followed by a nomToken of kTypeYl, such as "yl", "penta" is identified as referring to an alkyl chain, an appropriate connection table is constructed, and the nomToken is converted to

kTypeRoot, which is described above. In a different environment, when followed by a nomToken of kTypeRoot, "penta" indicates that the root structure should be repeated, and its original designation as kTypePrefix is retained for later handling.

5 The following description is with respect to the example of "penta". A pentane structure is a string of 5 carbon atoms separated by single bonds, with a sufficient number of hydrogen atoms to make 4 attachments on each carbon:
CH3-CH2-CH2-CH2-CH3. This is an example of an atomic chain. Pentasilane is
a similar structure with silicon atoms instead of carbon atoms:
10 SiH3-SiH2-SiH2-SiH2-SiH3. This is an example of a heteroatomic chain. "Silane"
is the single molecule SiH4, where the central atom is connected to each of the
four surrounding atoms by a single bond. However, "pentasilane" is not
properly interpreted to mean arranging 5 individual silane molecules next to
each other to produce SiH4 SiH4 SiH4 SiH4 SiH4. On the other hand,
15 "hydroxide" refers to a single molecule OH-, where the negatively-charged
oxygen is connected to the hydrogen by a single bond, and "pentahydroxide" is
in fact properly interpreted to mean arranging 5 individual hydroxide molecules
next to each other to produce OH- OH- OH- OH- OH-.

20 Cyclic systems are created and aromatic rings are fused at this point in the
processing. As shown, the order of interpretation is important in the individual
sections as well as in the interpretation process as a whole. A name such as

"benzocyclooctene" implies that chains (kTypePrefix, treated as described above) are to be interpreted first and then are to be closed (kTypeCyclo) before being submitted for participation in ring fusions (kTypeBenzo).

At this point, portions have been identified within the greater set of name
5 fragments that correspond to structures known as "root" or "core" structures.

After the main root portions of the name are identified, the consolidation process continues with nomTokens that directly modify the main root portions.

Such directly modifying nomTokens generally correspond to grammatical prefixes and suffixes within the original input name. In at least one embodiment, many nomTokens representing traditional chemical functional groups are recognized at this stage, including acids in variations, radical suffixes such as "-yl," and prefixes of heterocyclic "aza" nomenclature. Since there are many text strings that correspond to multiple nomTokens for functional groups, it is advantageous to examine the environments carefully for details.
10

15 In the last stages of the consolidation process, multiple large groups are joined, so that typically, for example, ligands are joined to root structures, cations to anions, and esters to acids.

An attach-out map having at least one remaining entry is present at the end of the consolidation process for a name such as "methyl" that is usually
20 intended to be joined to another name fragment. An appropriate radical is added to the connection table for such remaining entry in the attach-out map, wherein,

for example, "methyl" is a monoradical and "methyldene" is a diradical.

The consolidated list of nomTokens is examined for any remaining nomTokens of type kTypeUnknown having names that correspond to known stereochemical indicators (step 1080). Stereochemistry is considered at this point because stereochemistry may be determined by the entire contents of a connection table. If a suitable nomToken is found, the appropriate stereochemistry is added to the connection table, and the nomToken representing the stereochemical indicator is removed (step 1090).

As shown, each action following the fragmentation of the original input name has attempted to reduce the number of nomTokens in the resulting list. If the list has been reduced by this point to a single nomToken, the nomToken's connection table, if present, represents the structure corresponding to the original input name. In such a case, a representation of the structure (e.g., an image of the structure) is derived from the connection table and is presented to the user (step 1100). (See, e.g., the above-cited simultaneously filed application.) If more than one nomToken is present, or if the single nomToken lacks a connection table, it is determined that the original input name is uninterpretable and an appropriate error message is presented instead (step 1110).

An example using a specific chemical name is now described. A name "Phenacyl bromide, p-napthoxy" is submitted for processing. The name is preprocessed, including being converted to all lowercase characters, resulting in

"phenacyl bromide, p-napthoxy". A common typographical error "napt" is converted to "naphth", which produces "phenacyl bromide, p-naphthoxy". The name is uninverted, leaving "p-naphthoxy-phenacyl bromide".

The name is divided into six recognized fragments and a list of six corresponding nomTokens is created. These six nomTokens, with their types, subtypes, previous characters, and a graphical depiction of their connection tables, are shown in Fig. 7A.

The list of nomTokens is examined for recognized environments. The first recognized environment is found when the list is examined for amino acids. No amino acids are found in the list, but one nomToken ("yl") of type kTypeEnderAminoAcid is present. Such a nomToken, being meaningful only in the context of amino acids, is not meaningful in this list that contains no amino acids. Accordingly, the nomToken of type kTypeEnderAminoAcid is converted to the next-highest-ranked nomToken of identical name, which in this case is of type kTypeSuffix and subtype kSubtypeY1 (see Fig. 7B).

The next recognized environment is found in preparing to create ortho/peri fused ring systems. One example of such an environment requires, among other things, adjacent tokens of types kTypeOPFuser and kTypeRoot. In this list of nomTokens, a nomToken of type kTypeOPFuser exists but is followed by a nomToken of type kTypeInfix instead. Therefore, the nomToken of type kTypeOPFuser is determined not to be meaningful in this context, and is

converted to the next-highest-ranked nomToken of the same name, which in this case is of type kTypeRoot and subtype kSubtypeUnknown (see Fig. 7C).

The list is examined for nomTokens of type kTypeSuffix. Such a nomToken ("yl") is found, and is found to be preceded by a nomToken of type kTypeRoot, which results in a recognized environment. With respect to this recognized environment, an entry is added to the attach-out map of the root structure. In the absence of an explicit locant, the attach-out is assigned to the first atom in the connection table that has sufficient valences, which in this case is the terminal carbon (see Fig. 7D in which the attach-out is represented by a black diamond). The nomToken of kTypeSuffix is removed from the list, leaving five nomTokens in the list.

One of the nomTokens remaining in the list ("bromide") had been preceded by a space character in the preprocessed name. The space character may be chemically significant and is processed at this point. The list is divided into two smaller sublists, one of which contains the four nomTokens before the "bromide" nomToken, and the other of which contains the "bromide" nomToken only.

The first of the sublists is examined for nomTokens of type kTypeInfix. In this case, one nomToken of this type, "oxy", is found, and is preceded by another nomToken of type kTypeRoot, which results in a recognized environment. In this environment, the entire contents of the connection table of the kTypeInfix

nomToken are merged into the connection table of the root. Additionally, a bond is created between the first atoms with sufficient free valences originating in the two connection tables. Any entries (one in this case) in the attach-in and attach-out maps of the nomToken of type kTypeInfix are copied to corresponding atoms in the merged connection table. The subtype of the root structure is changed to kSubtypeInfix. The nomToken of type kTypeInfix is then discarded.

5 The second of the sublists is similarly examined, but no changes are necessary in this case. At this point, the entire list has four nomTokens (see Fig. 7E).

In this example, only one other environment is recognized in the sublists, and is found in the first sublist. The first sublist contains a nomToken of kTypeRoot ("phenacyl") that is preceded by another nomToken of kTypeRoot ("naphthoxy") that has exactly one entry in its attach-out list. Furthermore, the further preceding nomToken is of type kTypeUnknown and has a name ("p") that corresponds exactly to one of the entries in the locant map of "phenacyl".

10 Therefore, the connection tables for "naphthoxy" and for "phenacyl" are combined, and a bond is indicated between the atom referenced in the attach-out map of "naphthoxy" and the atom referenced by the "p" entry in the locant map for "phenacyl". Accordingly, with respect to the three nomTokens involved, two are discarded and the resulting connection table is stored in the third, which

15 leaves two nomTokens in the entire list (Fig. 7F), with exactly one nomToken in each sublist. As no other environments are recognized in either sublist, the two

sublists are recombined.

The last environment that is recognized consists of a nomToken of type kTypeCounterion following a nomToken of type kTypeRoot, each of which nomToken has at least one entry in its respective attach-out list. In this
5 environment, the two connection tables are merged, and a bond is indicated between the two atoms referenced by the attach-out lists (Fig. 7G).

At this point, the list has a single nomToken, which is of type kTypeRoot and has a non-empty connection table. As the attach-out list has no entries, no
10 radicals need to be added to the connection table. The name has been fully parsed. The structure shown in Fig. 7G is the correct structure for the original
name “phenacyl bromide, p-napthoxy”, and is presented to the user.

All or a portion of the procedures described above may be implemented in hardware or software, or a combination of both. In at least some cases, it is advantageous if the technique is implemented in computer programs executing
15 on one or more programmable computers, such as a personal computer running or able to run an operating system such as UNIX, Linux, Microsoft Windows 95, 98, 2000, or NT, or MacOS, that each include a processor, a storage medium readable by the processor (including volatile and non-volatile memory and/or
storage elements), at least one input device such as a keyboard, and at least one
20 output device. Program code is applied to data entered using the input device to perform the technique described above and to generate output information. The

output information is applied to one or more output devices such as a display screen of the computer.

In at least some cases, it is advantageous if each program is implemented in a high level procedural or object-oriented programming language such as Perl, C, C++, or Java to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

In at least some cases, it is advantageous if each such computer program is stored on a storage medium or device, such as ROM or optical or magnetic disc, that is readable by a general or special purpose programmable computer for configuring and operating the computer when the storage medium or device is read by the computer to perform the procedures described in this document. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner.

Other embodiments are within the scope of the following claims. For example, the system may be combined with one or more external databases of names and structures, so that a chemical name present in the external databases but not otherwise parsable would still produce a structure. In another example, non-English chemical names could be interpreted as well or instead. In another

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example, the fragmentation of the initial chemical name may be varied, e.g., by using different or extended lists of known chemical name fragments.

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What is claimed is:

Claims

1. A method for use in deriving chemical structural information,
comprising:
parsing a chemical name into at least first and second fragments; and
determining, based at least in part on the positions of the first and second
fragments within the chemical name, respective first and second diagrammatic
representations of the first and second fragments.

2. The method of claim 1, further comprising:
identifying, among a preselected set of text strings, respective first and
second text strings that correspond to the first and second fragments; and
basing the determination of the first and second diagrammatic
representations at least in part on conditions associated with the first and second
text strings.

3. A system for use in deriving chemical structural information,
comprising:
a parser parsing a chemical name into at least first and second fragments;
and
a determiner determining, based at least in part on the positions of the

first and second fragments within the chemical name, respective first and second diagrammatic representations of the first and second fragments.

4. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive chemical structural information, the instructions causing the system to:

parse a chemical name into at least first and second fragments; and
determine, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second diagrammatic representations of the first and second fragments.

DERIVING CHEMICAL STRUCTURAL INFORMATION

ABSTRACT OF THE DISCLOSURE

A method and a system are provided for deriving chemical structures from chemical names. Chemical name fragments are grouped into a number of classifications. The method and the system handle new and old chemical names, including names for organic and inorganic substances. The method and the system handle inverted names, including inverted names with missing commas or with extraneous spaces.

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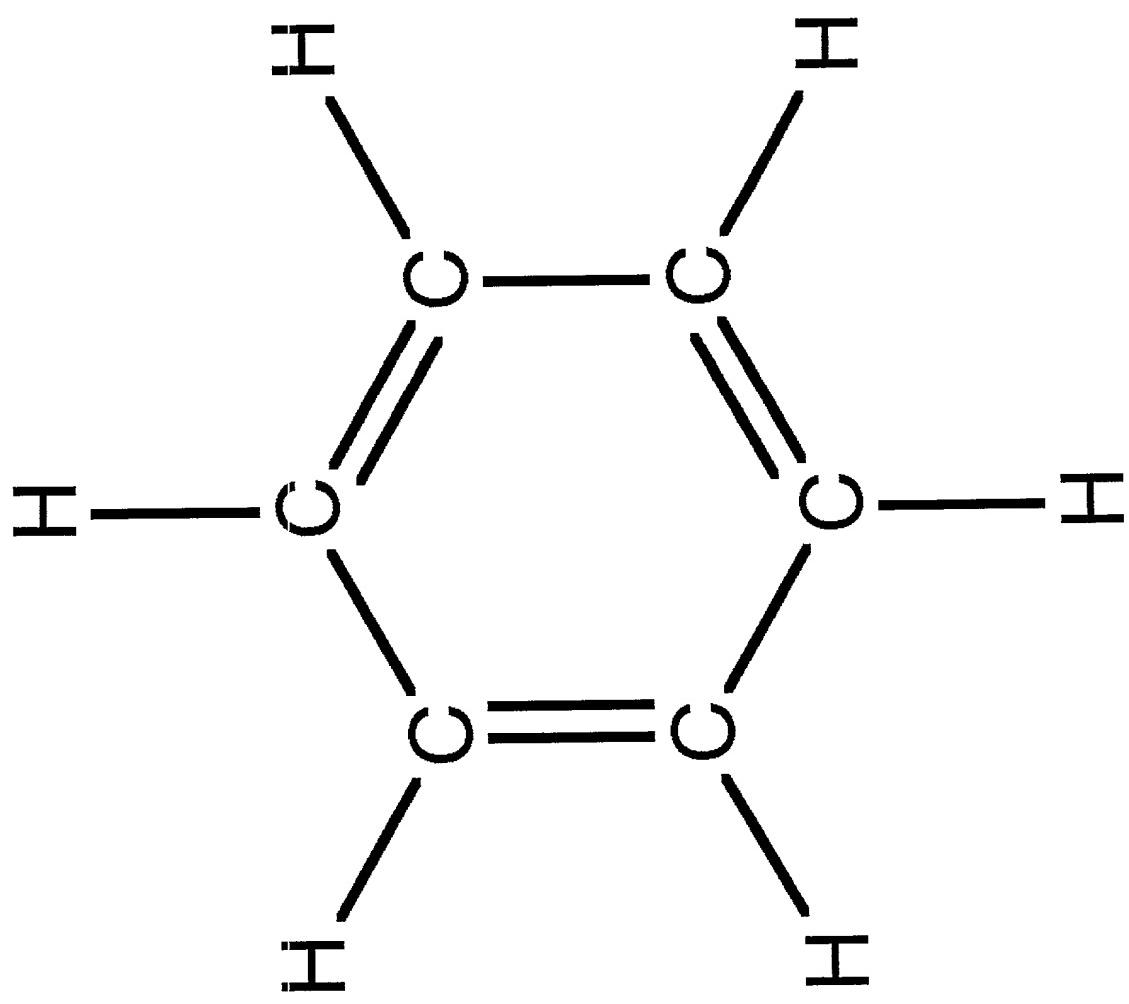


FIG. 1 (PRIOR ART)

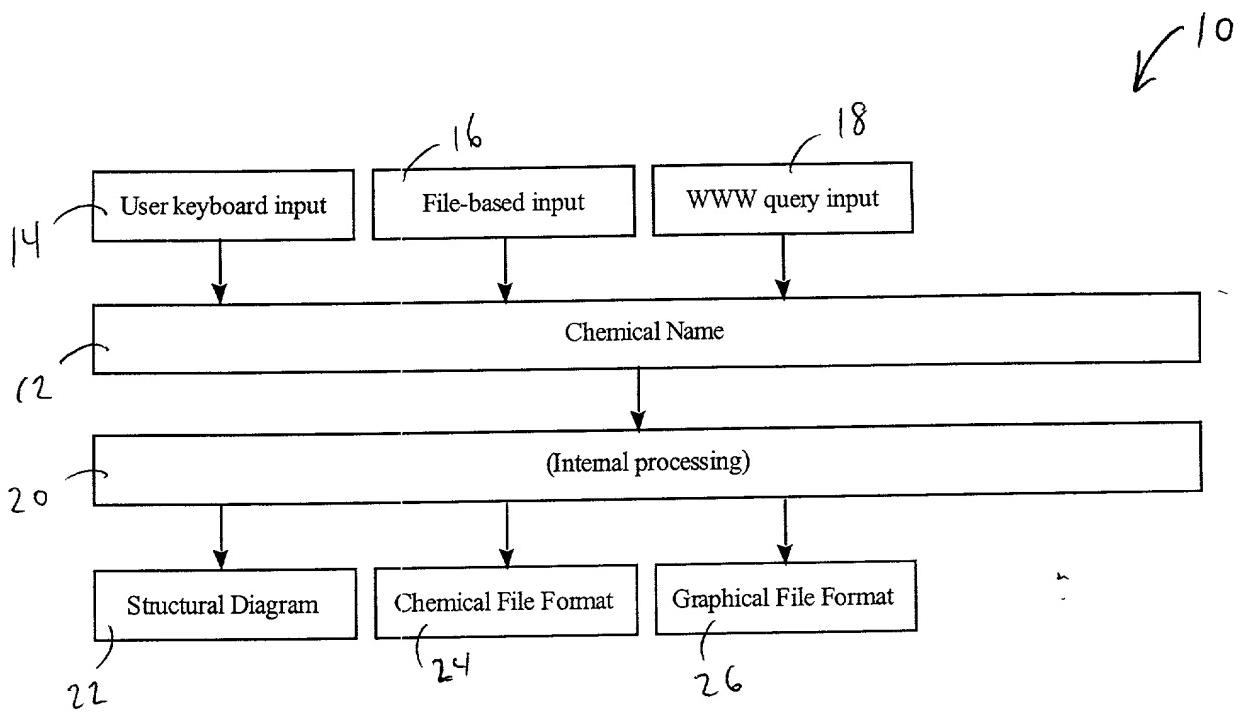


Fig. 2

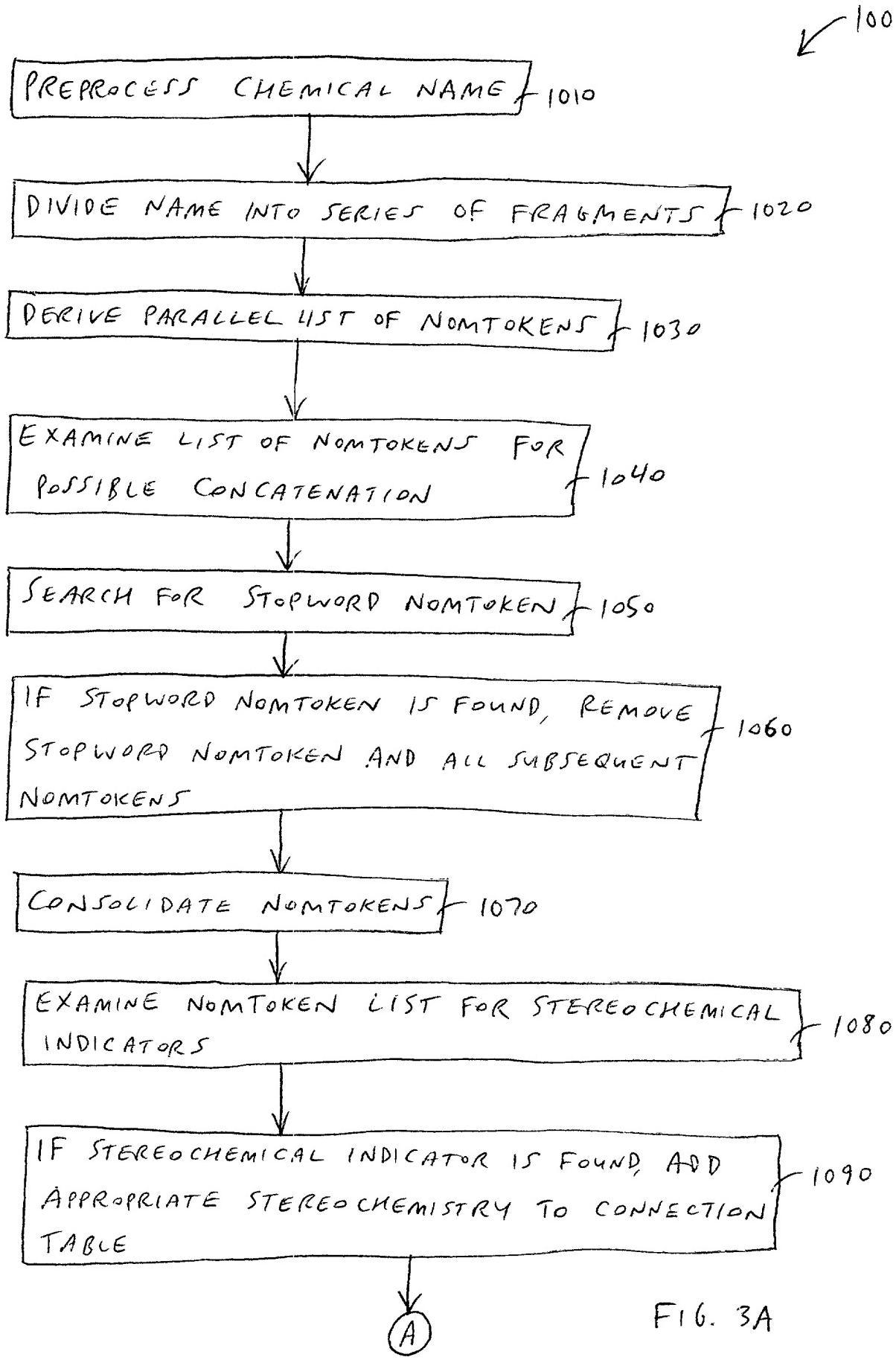


FIG. 3A

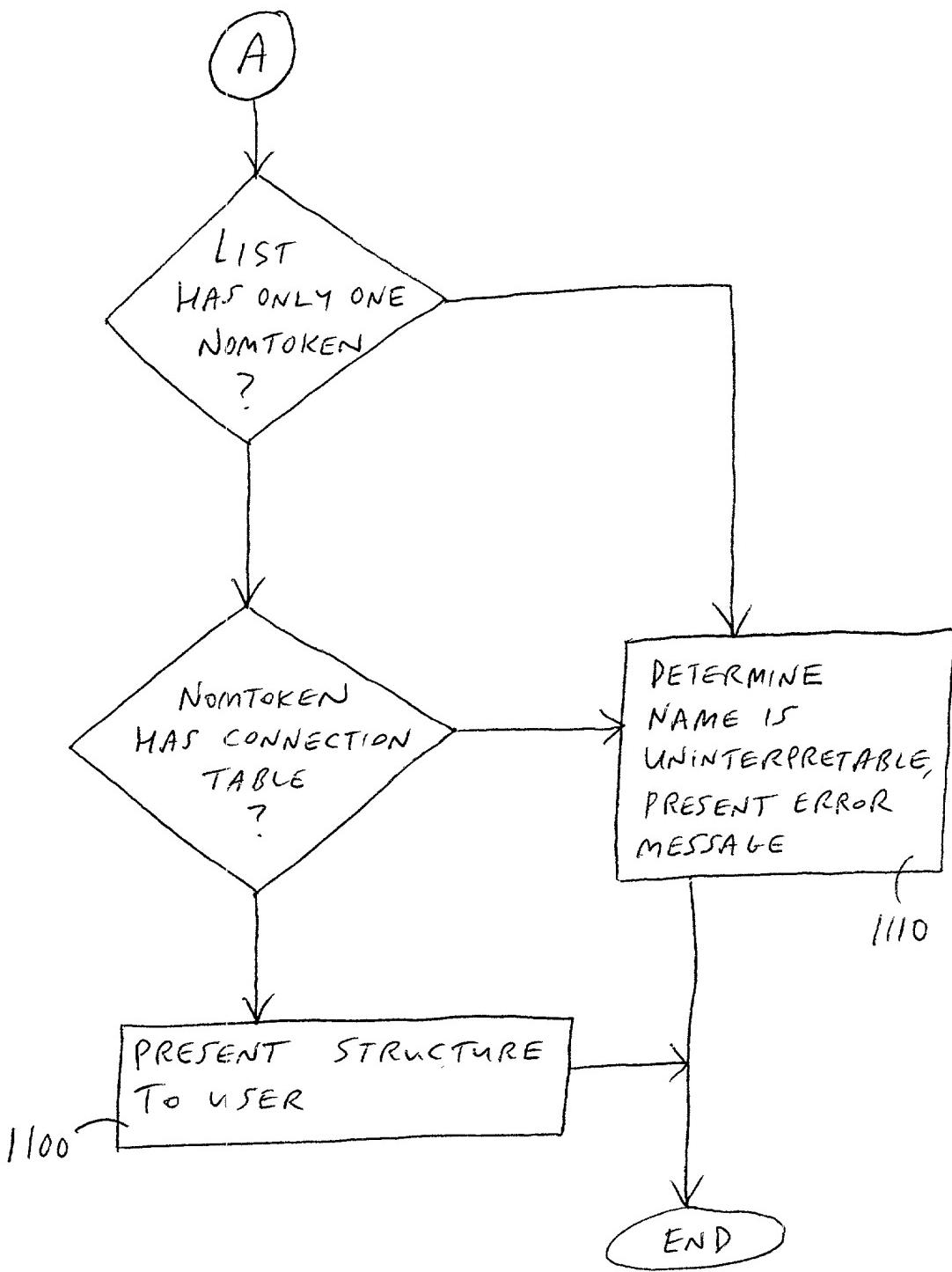


FIG. 3B

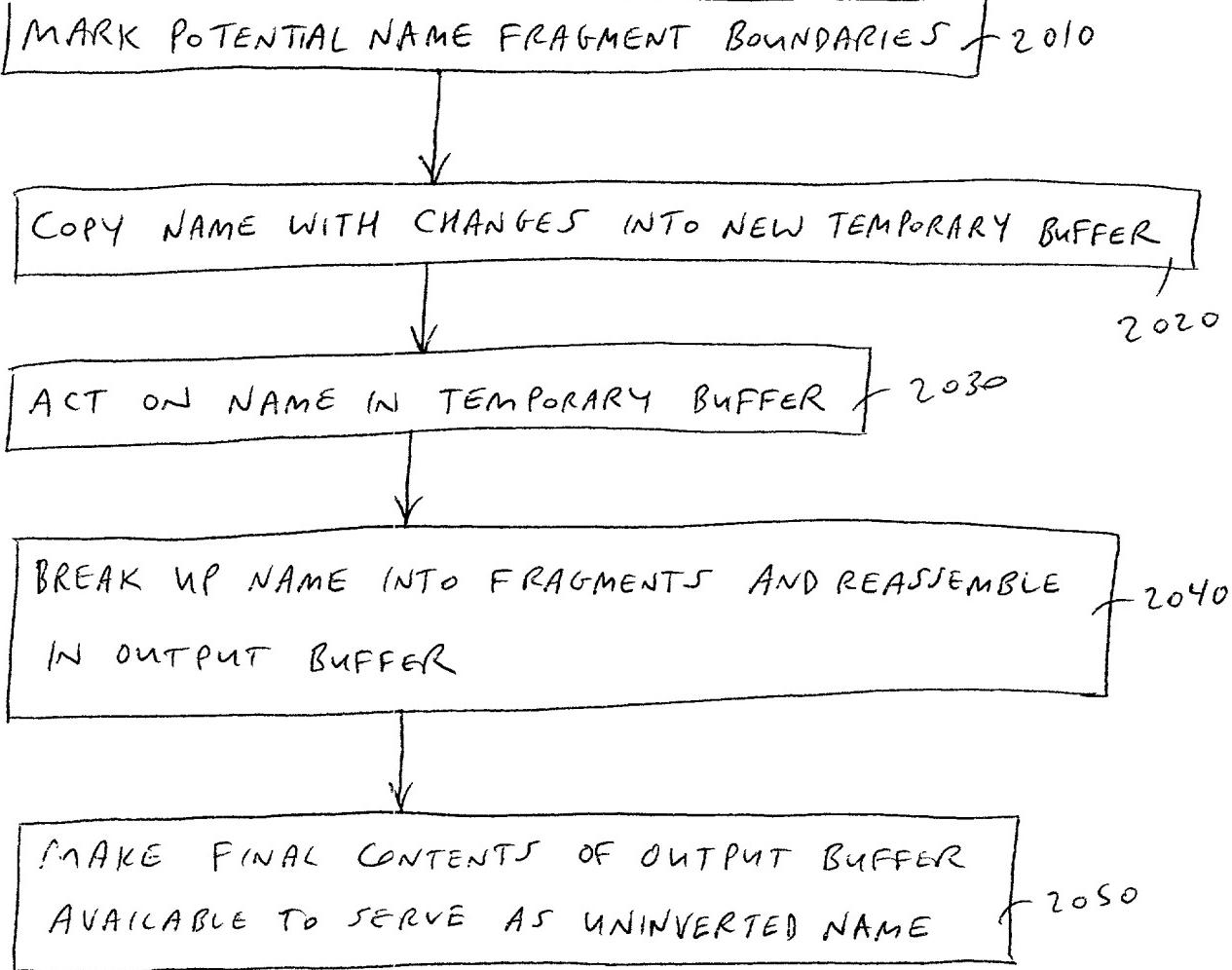


FIG. 4

Table 1: Strings that cannot terminate fragments to be prepended

"dry"
"ed"
"ide"
"ing"
"mm"
"one"
"rod"

FIG. 5A

Table 2: Strings that cannot initiate fragments to be prepended (note that some strings include a space character)

"in "
"ion"
"low "

FIG. SB

Table 3: Strings that cannot appear anywhere in fragments to be prepended (note that some strings include one or more space characters)

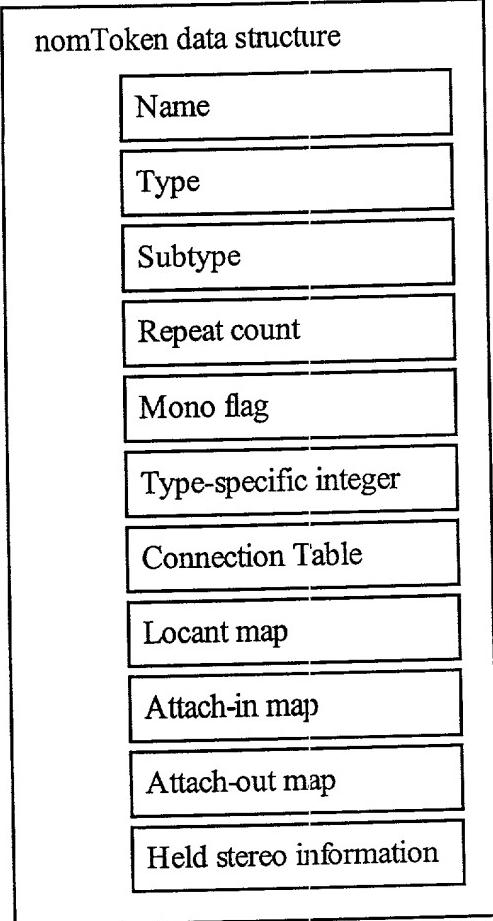
" and "	"grade"	"radical"
" in "	"granul"	"random"
" ion"	"grease"	"reagent"
"%"	"grit"	"reduc"
"/"	"hbr"	"regular"
"7ci"	"hcl"	"remainder"
"8ci"	"heavy"	"ribbon"
"9ci"	"hydrin"	"rods"
"10ci"	"hydrous"	"salt"
"aas"	"ide "	"scale"
"absolute"	"imine"	"shot"
"acid"	"ing"	"slug"
"acs"	"inhibit"	"soluble"
"aerosol"	"isotop"	"solution"
"amidine"	"ite"	"sphere"
"analy"	"ize"	"spong"
"approx"	"lactam"	"stab"
"assay"	"lacton"	"stabil"
"ate"	"light"	"standard"
"balance"	"lump"	"stick"
"basic"	"mainly"	"sublim"
"basis"	"medium"	"sultam"
"bead"	"mesh"	"sulton"
"briquette"	"micron"	"synthetic"
"catal"	"ml"	"syrup"
"certif"	"mm "	"tablet"
"chip"	"moist"	"tech"
"chunk"	"morphous"	"tion"
"cm"	"mossy"	"titrant"
"coarse"	"natural"	"tone"
"contain"	"needle"	"typic"
"crucible"	"neutral"	"usp"
"cryst"	"nitrile"	"wire"
"deriv"	"pearl"	"with"
"dispers"	"pellet"	"xime"
"dry "	"piece"	"zone"
"dust"	"plate"	
"ed "	"poly"	
"electro"	"porous"	
"ester"	"powder"	
"ether"	"ppm"	
"fcc"	"pract"	
"fine"	"predomina"	
"flake"	"predominantly"	
"foil"	"protected"	
"for "	"puratronic"	
"from"	"pure"	
"glacial"	"purity"	
	"purum"	

Table 4.

ether
sulfide
disulfide
trisulfide
tetrasulfide
pentasulfide
hexasulfide
selenide
diselenide
triselenide
telluride
sulfone
disulfone
trisulfone
sulfoxide
disulfoxide
~~trisulfoxide~~
peroxide
ketone
diketone
triketone
tetraketone

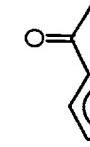
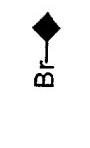
F16. SD

nomToken data structure



F16. 6

CONNECTION
TABLE

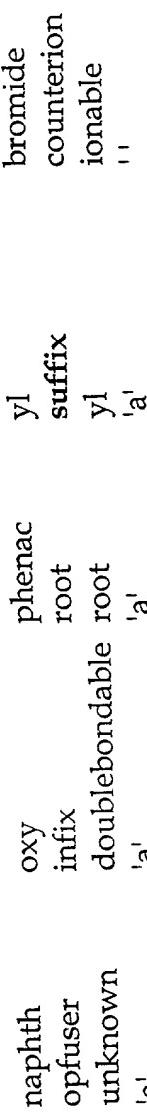
				
NAME	p	naphth	oxy	bromide
TYPE	unknown	opfuser	infix	counterion
SUBTYPE	unknown	unknown	doublebondable	ionable
PREV CHAR	('	'a'	'a'	'a'

F16. 7A

CONNECTION TABLE



The image displays three chemical structures. The first is 4-phenylacetone, consisting of a benzene ring attached to a carbonyl group (C=O) which is further attached to a methyl group (CH₃). The second is 4-hydroxyacetophenone, similar to the first but with a hydroxyl group (OH) instead of the methyl group. The third is naphthalene, which consists of two fused benzene rings.



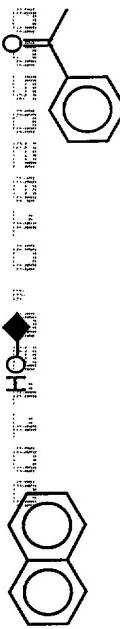
bromide counterionable



Fig. 7B

Br

CONNECTION
TABLE



NAME	P	naphth	oxy	yl
TYPE	unknown	root	infix	suffix

SUBTYPE	unknown	unknown	doublebondable	root	ionable
PREV CHAR	'('a'	'a'	'a'	'a'

SUBTYPE	unknown	unknown	doublebondable	root	ionable
PREV CHAR	'('a'	'a'	'a'	'a'

F16, 7C

Br

bromide
counterion

SUBTYPE	unknown	unknown	doublebondable	root	ionable
PREV CHAR	'('a'	'a'	'a'	'a'

SUBTYPE	unknown	unknown	doublebondable	root	ionable
PREV CHAR	'('a'	'a'	'a'	'a'

CONNECTION
TABLE

NAME	P	naphth	oxy
TYPE	unknown	root	infix
SUBTYPE	unknown	unknown	doublebondable
PREV CHAR	'('a'	'a'

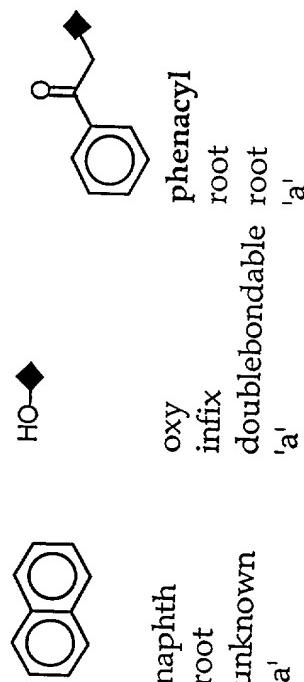


Fig. 7D

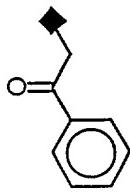
CONNECTION
TABLE

NAME	P
TYPE	unknown
SUBTYPE	unknown
PREV CHAR	'(



NAME	P
naphthoxy	root
	infix
	'a'

F16.7E

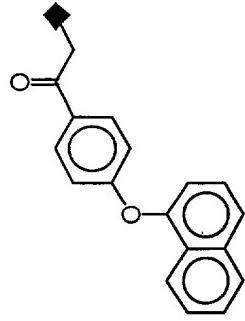


NAME	P
phenacyl	root
	root
	'a'



NAME	P
bromide	counterion
	ionable
	'1'

CONNECTION
TABLE



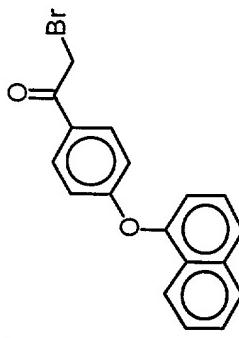
NAME p-naphthoxyphenacyl
TYPE root
SUBTYPE root
PREV CHAR 'a'

Br◆

bromide
counterion
ionable
--

FIG. 7F

CONNECTION
TABLE



NAME	p-naphthoxy-phenacyl bromide
TYPE	root
SUBTYPE	root
PREV CHAR	'a'

F16. 76

DECLARATION AND POWER OF ATTORNEY
(Attorney Docket No. 103544.127)

As a below-named inventor, I hereby declare that:

My residence, post office address and citizenship is as stated below next to my name.

I believe that I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled:

DERIVING CHEMICAL STRUCTURAL INFORMATION

the specification of which (check only one):

is attached hereto.

was filed as United States Patent Application
Serial No. _____
and was amended
on _____
(if applicable)

was filed as PCT Patent Application
Serial No. _____
on _____
and was amended under PCT Article 19
on _____
(if applicable)

I hereby state that I have reviewed and understand the contents of the above-identified specification, including the claims, as amended by any amendment referred to above.

I acknowledge the duty to disclose information which is material to the patentability of the claims of this application in accordance with Title 37, Code of Federal Regulations, Sections 1.56(a) and 1.56(b).

I hereby claim foreign priority benefits under Title 35, United States Code, §119(a)-(d) or 365(b) of any foreign application(s) for patent or inventor's certificate or of any PCT international application(s) designating at least one country other than the United States of America listed below and have also identified below any foreign application(s) for patent or inventor's certificate or any PCT international application(s) designating at least one country other than the United States of America filed by me on the same subject matter having a filing date before that of the application(s) of which priority is claimed:

EXPRESS MAIL LABEL NO. EM259723548US
DATE OF DEPOSIT February 11, 2000

**PRIOR FOREIGN/PCT APPLICATION(S) AND ANY PRIORITY CLAIMS
UNDER 35 U.S.C. §119(a)-(d) or 365(b):**

COUNTRY (if PCT indicate PCT)	APPLICATION NUMBER	DATE OF FILING	PRIORITY CLAIMED UNDER 35 U.S.C. §119(a)-(b) or 365(b) (YES/NO)
--	---------------------------	-----------------------	--

I hereby claim the benefit under 35 U.S.C. §119(e) of any United States provisional patent application(s) listed below:

APPLICATION NUMBER	DATE OF FILING	STATUS: (PENDING OR ABANDONED)
60/119,930	February 12, 1999	PENDING

I hereby claim the benefit under Title 35, United States Code, § 120 or 365(c) of any United States application(s) or PCT international application(s) designating the United States of America that is/are listed below and, insofar as the subject matter of each of the claims of this application is not disclosed in that/those prior application(s) in the manner provided by the first paragraph of Title 35, United States Code, § 112. I acknowledge the duty to disclose material information as defined in Title 37, Code of Federal Regulations, § 1.56 which occurred between the filing date of the prior applications and the national or PCT international filing date of this application:

**PRIOR U.S. APPLICATION OR PCT INTERNATIONAL APPLICATION(S)
DESIGNATING THE U.S. FOR BENEFIT UNDER 35 U.S.C. § 120 or 365(c):**

APPLICATION NUMBER	DATE OF FILING (day, month, year)	STATUS: (PATENTED, PENDING OR ABANDONED)
---------------------------	--	---

POWER OF ATTORNEY: As named inventors, we hereby appoint the following attorneys and/or agents to prosecute this application and transact all business in the Patent and Trademark Office connected therewith

Michael J. Bevilacqua	Reg. No. 31,091
James E. Lampert	Reg. No. 24,564
Wayne M. Kennard	Reg. No. 30,271
Hollie L. Baker	Reg. No. 31,321
Wayne A. Keown	Reg. No. 33,923
Donald R. Steinberg	Reg. No. 37,241
Michael A. Diener	Reg. No. 37,122
Richard A. Goldenberg	Reg. No. 38,895

Peter M. Dichiara	Reg. No. 38,005
Ann-Louise Kerner	Reg. No. 33,523
Colleen Superko	Reg. No. 39,850
Gretchen Rice	Reg. No. 37,429
Keum J. Park	Reg. No. 42,059
Jason A. Reyes	Reg. No. 41,513
Janice M. Klunder	Reg. No. 41,121
Henry N. Wixon	Reg. No. 32,073
Barbara A. Barakat	Reg. No. 32,190
Nancy Chiu	Reg. No. 43,545
Rajesh Vallabh	Reg. No. 35,761
Ayla A. Lari	Reg. No. 43,739

the mailing address and telephone number of each of whom is HALE AND DORR LLP, 60 State Street, Boston, Massachusetts 02109 and (617) 526-6000, with full power of substitution and revocation to prosecute this application and to transact all business in the Patent and Trademark Office connected therewith.

Send Correspondence To

**Jason A. Reyes
Hale and Dorr LLP
60 State Street
Boston, MA 02109**

Direct Telephone Calls To

**Jason A. Reyes
(617) 526-6010**

Wherefore I petition that letters patent be granted to me for the invention or discovery described and claimed in the attached specification and claims, and hereby subscribe my name to said specification and claims and to the foregoing declaration, power of attorney, and this petition.

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

Full name of sole inventor: Jonathan S. Brecher

Inventor's signature _____ Date _____

Country of Citizenship: USA

Residence: 52 Montgomery Street, #2, Cambridge, MA 02140

Post Office Address: _____

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant: Jonathan Scott Brecher

Serial No.: To Be Assigned

Filed: Herewith (This application claims the benefit of U.S. Provisional Application Serial No. 60/119,930 entitled DERIVING A CHEMICAL STRUCTURE FROM A CHEMICAL NAME, filed on February 12, 1999.)

Title: DERIVING CHEMICAL STRUCTURAL INFORMATION

Box Patent Application
Assistant Commissioner for Patents
Washington, DC 20231

COVER SHEET FOR APPENDIX: NOMTOKENS

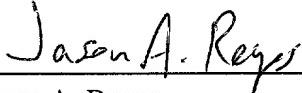
Dear Sir:

Enclosed for filing in the above-referenced patent application is the following document:

1. Appendix: NOMTOKENS, 111 pages.

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Respectfully submitted,



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Dated: February 11, 2000

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meth|carbin root alkane C,a|alpha|1|w|omega
carbenium root root [C+],1|w|omega
carbene root root C,32@1|w omega
aminylene|nitrene root root N,32@1|w|omega
hydroxymethyl root root C,4@x,O,x
hydroxymethylene root root C,8@x,O,x
form root trivial C,x|1|w|omega,(=O),x
formimino root trivial C,4@x|1|w|omega,(=N),x
formalin root root C=O,x
eth root alkane C,1|a|alpha,C,2|b|beta|w|omega
ethene|ethen root alkane C,1|a|alpha,=,x,C,2|b|beta|w|omega
ethyne|ethyn root alkane C,1|a|alpha,#,x,C,2|b|beta|w|omega
acet root trivial C,1,(=,x,O,x,),x,C,2|a|alpha|w|omega
aceto root trivial C,4@1,(=,x,O,x,),x,C,2|a|alpha|w|omega
acetoacet|acetoaceto root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3,(=,x,O,x,),x,C,4|g|gamma|w|omega
prop|propa root alkane C,1|a|alpha,C,2|b|beta,C,3|g|gamma|w|omega
isoprop|isopropa|isopropion root alkane C,a|alpha,(,x,C,b|beta,),x,C,x
hexafluoroisoprop|hexafluoroisopropa root alkane
C,a|alpha,(C(F)(F)F),x,C(F)(F)F,x
propiono|propion|propio|propri root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta|w|omega
proparg|proparag root alkane C,1|a|alpha,C,2,#,x,C,3|w|omega
tetroil loveracid alkane C,1,C,2,#,x,C,3,C,4|w|omega
but|buta root alkane C,1|a|alpha,C,2|b|beta,C,3|g|gamma,C,4|d|delta|w|omega
butyro|butyr root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma|w|omega
isobutyro|isobutyr root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(,x,C,3|b|beta,),x,C,4|b'|beta'|g|gamma|w|omega
isobutylene root root C=C(C)C,x
crotono|croton root trivial
C,1,(=,x,O,x,),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
crot root root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
crotonylalcohol root root
C,1,(0),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
isocrotono|isocroton root trivial
C,1,(=,x,O,x,),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
isocrot root root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
seneci root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,=,x,C,3|b|beta,(,x,C,4|g|gamma|w|omega,),x,C,4'|g'|
gamma'|w'|omega'
tigl|cevad root trivial
C,1,(=,x,O,x,),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
angel root trivial
C,1,(=,x,O,x,),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
pren root alkane C,1,C,2|a|alpha,=,x,C,3|b|beta,(C),x,C,4|g|gamma|w|omega
valero|valer|valerian root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
acetoxonal root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(=O),x,C,3|b|beta,C,4|g|gamma,(=O),x,C,5|d|delta|w|
omega
valpr root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(CCC),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
levulin|laevulin|levul root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4,(=O),x,C,5|g|gamma|d|delta|w|omega
isovalero|isovaler|delphin root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,(,x,C,4|g|gamma,),x,C,5|d|delta|w|omega

pival root trivial
 C,1,(=,x,O,x,),x,C,2|a|alpha,(,x,C,3|b|beta,) (,x,C,4|3',),x,C,5|3''
 amy1 root alkane C,4@1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
 capro root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon|w|omega
 acexam root root
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,N,x,C,x,(=O),x,
 C,x,
 enatho|enanth|oenantho|oenanth root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7|w|omega
 geron root trivial
 C,1,(=,x,O,x,),x,C,2|a|alpha,(C)(C),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|e
 psilon,(=O),x,C,7|w|omega
 capryl root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8|w|omega
 octoate root root
 O,1@x,C,1,(=O),x,C,2|a|alpha,(,x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilo
 n,),x,C,x,C,x
 pelargono|pelargon|pelarg|pergon root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9|w|o
 mega
 capr root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0|w|omega
 obtusil root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
 ,C,10|w|omega
 stilling root alkane
 C,1,/x,C,2|a|alpha,=,x,C,3|b|beta,/x,C,4|g|gamma,=,x,C,5|d|delta,\x,C,6|e|eps
 ilon,C,7,C,8,C,9,C,10|w|omega
 lauro|laur|vulg|laurostear root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12|w|omega
 linder root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
 ,C,10,C,11,C,12|w|omega
 myristo|myrist root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14|w|omega
 physeter|physoter root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,=,x,C,6|e|epsilon,C,7,C,8,C,9
 ,C,10,C,11,C,12,C,13,C,14|w|omega
 ipurol root alkane
 C,1,C,2|a|alpha,C,3|b|beta,(O),x,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
 ,9,C,10,C,11,(O),x,C,12,C,13,C,14|w|omega
 tsuzu|tudu root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
 ,C,10,C,11,C,12,C,13,C,14|w|omega
 myristelaid root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/x,C,9
 ,=,x,C,10,/x,C,11,C,12,C,13,C,14|w|omega
 myristole root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/x,C,9
 ,=,x,C,10,\x,C,11,C,12,C,13,C,14|w|omega
 palmito|palmit|cet root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16|w|omega

palmitelaid root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
 palmitole root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
 hiragon root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,=,x,C,7,C,8,C,9
 ,C,10,=,x,C,11,C,12,C,13,C,14,=,x,C,15,C,16|w|omega
 ustil root alkane
 C,1,C,2|a|alpha,(O),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
 ,9,C,10,C,11,C,12,C,13,C,14,C,15,(O),x,C,16|w|omega,O,x
 ambrettol root alkane
 C,1,C,2|a|alpha,(O),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,=,x,C
 ,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,O,x
 aleurit root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(O)
 ,x,C,10,(O),x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,O,x
 gaid|hypogae root alkane
 C,1,C,2|a|alpha,=,x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
 ,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
 juniper root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,O,x
 margaro|margar root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17|w|omega
 stear|stearophan root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 moroct root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,=,x
 ,C,9,C,10,C,11,C,12,=,x,C,13,C,14,C,15,=,x,C,16,C,17,C,18|w|omega
 parinar root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,=,x
 ,C,10,C,11,=,x,C,12,=,x,C,13,=,x,C,14,\,x,C,15,C,16,C,17,C,18|w|omega
 eleostear root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,=,x,C,12,/,x,C,13,=,x,C,14,\,x,C,15,C,16,C,17,C,18|w|omega
 stearol loveracid root
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,#,x
 ,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 couep|lican root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,(=O),x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,
 C,9,=,x,C,10,C,11,=,x,C,12,C,13,=,x,C,14,C,15,C,16,C,17,C,18|w|omega
 trichosan root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,=,x,C,12,\,x,C,13,=,x,C,14,/,x,C,15,C,16,C,17,C,18|w|omega
 floionol|phloionol root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(O)
 ,x,C,10,(O),x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega,O,x
 lycaon root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,(=O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 lactarin root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,(=O),x,C,7,C,8,
 C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

jalapinol root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,(O),x,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 ole root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 elaid root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 ricinole|ricinol root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 ricinelaid root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 linole|telfair root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,/,x,C,12,=,x,C,13,\,x,C,14,C,15,C,16,C,17,C,18|w|omega
 vernal loveracid root CCCCCCCC\=C=C/C[C@H]1[C@H](CCCCC)O1,x
 linolelaid root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,/,x,C,12,=,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega
 linolenelaid root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,/,x,C,12,=,x,C,13,/,x,C,14,/,x,C,15,=,x,C,16,/,x,C,17,C,18|w|
 omega
 linolen|alphanolinolen root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,/,x,C,12,=,x,C,13,\,x,C,14,/,x,C,15,=,x,C,16,\,x,C,17,C,18|w|
 omega
 gammalinolen root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,=,x,C,7,\,x
 ,C,8,/,x,C,9,=,x,C,10,\,x,C,11,/,x,C,12,=,x,C,13,\,x,C,14,C,15,C,16,C,17,C,18|w|
 omega
 vaccen root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,/,x,C,11,=,x,C,12,/,x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 petroselaid root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,=,x,C,7,/,x
 ,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 petroselin root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,=,x,C,7,\,x
 ,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 calend root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,/,x,C,8,=,x
 ,C,9,\,x,C,10,=,x,C,11,\,x,C,12,=,x,C,13,\,x,C,14,C,15,C,16,C,17,C,18|w|omega
 arachido|arachid|arachin root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega
 gadole root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega
 arachidon root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,/,x,C,5|d|delta,=,x,C,6|e|epsilon,\,x,C,7
 ,/,x,C,8,=,x,C,9,\,x,C,10,/,x,C,11,=,x,C,12,\,x,C,13,/,x,C,14,=,x,C,15,\,x,C,16,
 C,17,C,18,C,19,C,20|w|omega

arach root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21|w|omega
 lesquerol root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,/,x,C,11,=,x,C,12,\,x,C,13,[C@H],14,(O),x,C,15,C,16,C,17,C,18,C,19,C,20,C,21|w
 |omega
 beheno|behen root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22|w|omega
 eruc root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,/,x,C,13,=,x,C,14,\,x,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22|w|omeg
 a
 brassid root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,/,x,C,13,=,x,C,14,/,x,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22|w|omeg
 a
 lignocero|lignocer root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24|w|omega
 cerebron|phrenosin root alkane
 C,1,C,2|a|alpha,(O),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
 ,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24|w|
 omega
 nervon root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,/,x,C,15,=,x,C,16,\,x,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C
 ,24|w|omega
 hyen root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25|w|o
 mega
 cerotino|cerotin|cerot|cerane root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
 6|w|omega
 ceryl root alkane
 C,4@1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C
 ,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C
 ,26|w|omega
 cluyt|montano|montan root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
 6,C,27,C,28|w|omega
 melisso|meliss|myric root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
 6,C,27,C,28,C,29,C,30|w|omega
 laccero|lacer root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
 6,C,27,C,28,C,29,C,30,C,31,C,32|w|omega
 acroleine|acrolein root root C,1,(=,x,O,x,),x,C,2|a|alpha,=,x,C,3|b|beta|w|omega
 methacrolein root root C,1,(=,x,O,x,),x,C,2|a|alpha,(C),x,=,x,C,3|b|beta|w|omega
 acr root trivial C,1,(=,x,O,x,),x,C,2|a|alpha,=,x,C,3|b|beta|w|omega
 hydracr root trivial C,1,(=,x,O,x,),x,C,2,C,3|w|omega,O,o

methacr root trivial C,1,(=,x,O,x,),x,C,2,(,x,C,4,),x,=,x,C,3|w|omega
 propiol root trivial C,1,(=,x,O,x,),x,C,2,#,x,C,3
 glyoxal root trivial C,1,(=,x,O,x,),x,C,2,=,x,O,x
 oxalo|oxal root diacid C,1,(=,x,O,x,),x,C,4@2,=,x,O,x
 oxamid|oxam root trivial C,1,(=,x,O,x,),x,C,2,(,x,N,n,),x,=,x,O,x
 oxanil root trivial
 C,1,(=,x,O,x,),x,C,2,(,x,N,n,c,1',Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Ring1
 ,),x,=,x,O,x
 mucochlor root trivial
 C,1,(=,x,O,x,),x,C,2|a|alpha,(Cl),x,=,x,C,3|b|beta|w|omega,(Cl),x,C=O,x
 mucobrom root trivial
 C,1,(=,x,O,x,),x,C,2|a|alpha,(Br),x,=,x,C,3|b|beta|w|omega,(Br),x,C=O,x
 pyromuc root root C,x,c,x,Ring,Ring1,c,x,c,x,c,x,o,x,Ring,Ring1
 malono|malon root diacid C,1,(=,x,O,x,),x,C,2|w|omega,C,4@3,=,x,O,x
 tartrono|tartron root diacid C,1,(=,x,O,x,),x,C,2,(,x,O,x,),x,C,4@3,=,x,O,x
 mesoxal root diacid C,1,(=,x,O,x,),x,C,2,(=,x,O,x,),x,C,4@3,=,x,O,x
 mesoxalo root root C,4@1,(=,x,O,x,),x,C,2,(=,x,O,x,),x,C,3,(,x,O,x,),x,=,x,O,x
 oxalacet root diacid
 C,1,(=,x,O,x,),x,C,2|a|alpha,C,3,(=,x,O,x,),x,C,4@4|w|omega,=,x,O,x
 oxalaceto root diacid
 C,4@1,(=,x,O,x,),x,C,2|a|alpha,C,3,(=,x,O,x,),x,C,4,(,x,O,x,),x,=,x,O,x
 succino|succin root diacid C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4@4,=,x,O,x
 isosuccino|isosuccin root diacid
 C,1,(=,x,O,x,),x,C,2|a|alpha,(,x,C,3|b|beta,),x,C,4@4,=,x,O,x
 caron root diacid
 C,1,(=,x,O,x,),x,C,2|a|alpha,(C(C)(C),x,Ring,Ring1,),x,C,3|b|beta,Ring,Ring1,C,4
 @4,=,x,O,x
 male|malen|malein|toxil root diacid
 C,1,(=,x,O,x,),x,/,x,C,2,=,x,C,3,\,x,C,4@4,=,x,O,x
 fumar|bolet root diacid C,1,(=,x,O,x,),x,/,x,C,2,=,x,C,3,/,x,C,4@4,=,x,O,x
 maleur root trivial C,1,(=,x,O,x,),x,/,x,C,2,=,x,C,3,\,x,C,4,N,x,C,x,(=O),x,N,x
 citracon root diacid C,1,(=,x,O,x,),x,/,x,C,2,(C),x,=,x,C,3,\,x,C,4@4,=,x,O,x
 mesacon root diacid C,1,(=,x,O,x,),x,/,x,C,2,(C),x,=,x,C,3,/,x,C,4@4,=,x,O,x
 teracon root diacid C,1,(=,x,O,x,),x,C,2,(=C(C)C),x,C,3,C,4@4,=,x,O,x
 mal root diacid C,1,(=,x,C,x,),x,C,2,(,x,O,x,),x,C,3,C,4@4,=,x,O,x
 citramal root diacid C,1,(=,x,O,x,),x,C,2,(,x,O,x,)(,x,C,x,),x,C,3,C,4@4,=,x,O,x
 pyrotartr|pyrotartar root diacid
 C,1,(=,x,O,x,),x,C,2,(,x,C,x,),x,C,3,C,4@4,=,x,O,x
 itacon root diacid C,1,(=,x,O,x,),x,C,2,(=,x,C,x,),x,C,3,C,4@4,=,x,O,x
 tartar|tartr|dtartar|dtartr|uv|mesotartar|mesotartr pseudosugar unknown x,x
 tartar|tartr|uv root diacid
 C,1,(=O),x,Ring,Ring1,,x,O,o,Ring,Ring2,,x,O,o',Ring,Ring3,,x,C,2,Ring,Ring1,
 Ring,Ring2,C,3,Ring,Ring3,C,4@4,=,x,O,x
 dtartar|dtartr root diacid
 C,1,(=O),x,Ring,Ring1,,x,O,o,Ring,Ring2,,x,O,o',Ring,Ring3,,x,[C@H],2,Ring,Ri
 ng1,Ring,Ring2,[C@H],3,Ring,Ring3,C,4@4,=,x,O,x
 ltartar|ltartr root diacid
 C,1,(=O),x,Ring,Ring1,,x,O,o,Ring,Ring2,,x,O,o',Ring,Ring3,,x,[C@@H],2,Ring,R
 ing1,Ring,Ring2,[C@@H],3,Ring,Ring3,C,4@4,=,x,O,x
 mesotartar|mesotartr root diacid
 C,1,(=O),x,Ring,Ring1,,x,O,o,Ring,Ring2,,x,O,o',Ring,Ring3,,x,[C@@H],2,Ring,R
 ing1,Ring,Ring2,[C@H],3,Ring,Ring3,C,4@4,=,x,O,x
 him root diacid
 C,x,(=,x,O,x,),x,C,2,Ring,Ring1,C,3,(,x,C,4,Ring,Ring2,C,5,=,x,C,6,C,1,(,x,C,7,R
 ing,Ring2,),x,Ring,Ring1,),x,C,4@X,=,x,O,x
 glutaro|glutar root diacid
 C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,4@5,=,x,O,x

adipo|adip root diacid
 $C,1,(=,x,O,x,),x,C,2|a|\alpha,C,3|b|\beta,C,4|g|\gamma,C,5|d|\delta,C,4@6,=,x,O,x$
 glutacon|glutacono root diacid $C,1,(=,x,O,x,),x,C,2,=,x,C,3,C,4,C,4@5,=,x,O,x$
 mucon|mucono root diacid $C,1,(=,x,O,x,),x,C,2,=,x,C,3,C,4,=,x,C,5,C,4@6,=,x,O,x$
 dihydromucon|dihydromucono root diacid
 $C,1,(=,x,O,x,),x,C,2,=,x,C,3,C,4,C,5,C,4@6,=,x,O,x$
 pimelo|pimel|piler root diacid
 $C,1,(=,x,O,x,),x,C,2,C,3,C,4,C,5,C,6,C,4@7,=,x,O,x$
 subero|suber root diacid
 $C,1,(=,x,O,x,),x,C,2|a|\alpha,C,3|b|\beta,C,4|g|\gamma,C,5|d|\delta,C,6,C,7,C,4@8,=,x,O,x$
 azela|azele|azel|leparcyl root diacid
 $C,1,(=,x,O,x,),x,C,2|a|\alpha,C,3|b|\beta,C,4|g|\gamma,C,5|d|\delta,C,6,C,7,C,8,C,4@9,=,x,O,x$
 sebaco|sebac root diacid
 $C,1,(=,x,O,x,),x,C,2|a|\alpha,C,3|b|\beta,C,4|g|\gamma,C,5|d|\delta,C,6,C,7,C,8,C,9,C,4@10,=,x,O,x$
 traumat|traumato root diacid
 $C,1,(=,x,O,x,),x,C,2,=,x,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,4@12,=,x,O,x$
 brassylo|brassyl root diacid
 $C,1,(=,x,O,x,),x,C,2|a|\alpha,C,3|b|\beta,C,4|g|\gamma,C,5|d|\delta,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,4@13,=,x,O,x$
 thapso|thaps root diacid
 $C,1,(=,x,O,x,),x,C,2|a|\alpha,C,3|b|\beta,C,4|g|\gamma,C,5|d|\delta,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,4@16,=,x,O,x$
 floion|phloion root diacid
 $C,1,(=,x,O,x,),x,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,(O),x,C,10,(O),x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,4@18,=,x,O,x$
 folin root diacid
 $C,x,(=,x,O,x,),x,(C(CC,x,C,4@x,=O)NC(C(C=C3)=CC=C3NCC(CN2)N(C=O)C1=C2N=C(N)NC1=O)=O),x$
 spiculspor root diacid
 $C,x,(=,x,O,x,),x,Ring,Ring1,..,x,C,1,(,x,=,x,O,x,),x,(,x,O,x,Ring,Ring2,),x,C,2,C,3,C,4,Ring,Ring2,Ring,Ring1,C,5,(,x,C,4@x,=,x,O,x,),x,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15$
 chaulmoogr root alkane
 $C,1,C,2|a|\alpha,C,3|b|\beta,C,4|g|\gamma,C,5|d|\delta,C,6|e|\epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,[C@H],x,Ring,Ring1,c,x,c,x,C,x,C,x,Ring,Ring1$
 pyrocarbon root diacid $C,x,(=,x,O,x,),x,O,x,C,4@x,=,x,O,x$
 imidodicarbon|iminodicarbon root diacid $C,x,(=,x,O,x,),x,N,n,C,4@x,=,x,O,x$
 pyrocarbon root diacid $C,x,(=,x,O,x,),x,O,x,C,4@x,=,x,O,x$
 thiodicarbon root diacid $C,x,(=,x,O,x,),x,S,x,C,4@x,=,x,O,x$
 peroxydicarbon root diacid $C,x,(=,x,O,x,),x,OO,x,C,4@x,=,x,O,x$
 thioperoxydicarbon root diacid $C,x,(=,x,O,x,),x,SS,x,C,4@x,=,x,O,x$
 chelidon|chelid root diacid $C,x,(=,x,O,x,),x,c1cc(=O)cc(o1),x,C,4@x,=,x,O,x$
 pamo|embon root diacid
 $C,x,(=,x,O,x,),x,C1=CC3=C(C=CC=C3)C(CC2=C(C=CC=C4)C4=CC(,x,C,4@x,=,x,O,x,)=C2O)=C1O,x$
 citr root polyacid $C,1,C,2,C,3,(,x,O,x,),x,(,x,C,x,),x,C,x,C,x$
 isocitr root polyacid $C,x,C,x,(,x,O,x,),x,C,x,(,x,C,x,),x,C,x,C,x$
 tricarballyl root polyacid $C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x$
 aconit root polyacid $C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x$
 trimellit root polyacid
 $C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,c,5,(,x,C,x,),x,c,6,Ring,Ring1$
 hemimellit root polyacid
 $C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,(,x,C,x,),x,c,4,c,5,c,6,Ring,Ring1$

hemimellitene root root
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,(,x,C,x,),x,c,4,c,5,c,6,Ring,Ring1
 pyromellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,(,x,C,x,),x,c,5,(,x,C,x,),x,c,6,Ring,Ring1
 pyromellitene root root
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,(,x,C,x,),x,c,5,(,x,C,x,),x,c,6,Ring,Ring1
 mellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(C),x,c,3,(C),x,c,4,(C),x,c,5,(C),x,c,6,(C),x,Ring,Ring1
 trimes root polyacid
C,x,c,1,Ring,Ring1,c,2,c,3,(,x,C,x,),x,c,4,c,5,(,x,C,x,),x,c,6,Ring,Ring1
 mellophan root polyacid
C,x,c,1,Ring,Ring1,c,2,(C),x,c,3,(C),x,c,4,(C),x,c,5,c,6,Ring,Ring1
 prehnit root polyacid
C,x,c,1,Ring,Ring1,c,2,(C),x,c,3,(C),x,c,4,c,5,(C),x,c,6,Ring,Ring1
 berberon|beron root polyacid
C,x,c,2,Ring,Ring1,c,3,(,x,C,x,),x,c,4,c,5,(,x,C,x,),x,c,6,n,1,Ring,Ring1
 phthalide root root
O,x,=,x,C,1,Ring,Ring1,O,2,C,3|a|alpha,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 phthalane|phthalan root root
C,1,Ring,Ring1,O,2,C,3,C,3a,Ring,Ring2,=,x,C,4,C,5,=,x,C,6,C,7,=,x,C,7a,Ring,Ring1,Ring,Ring2
 phthalo|phthal|orthophthal root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,(,x,C,4@x,=,x,O,x,),x,c,3,c,4,c,5,c,6,Ring,Ring1
 homophthalo|homophthal root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,(,x,C,x,C,4@x,=,x,O,x,),x,c,3,c,4,c,5,c,6,Ring,Ring1
 isophthalo|mphthalo|isophthal|mphthal root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,c,3,(,x,C,4@x,=,x,O,x,),x,c,4,c,5,c,6,Ring,Ring1
 terephthalo|pphthalo|terephthal|pphthal root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,C,4@x,=,x,O,x,),x,c,5,c,6,Ring,Ring1
 uvit root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,c,3,(,x,C,4@x,=,x,O,x,),x,c,4,c,5,(C),x,c,6,Ring,Ring1
 leucate|leucicacid root root
C,1,(=,x,O,x,),x,(,x,O,1@x,),x,C,2,(,x,O,x,),x,C,3,C,4,(,x,C,5,),x,C,x
 phenylephrine|phenylephrin root root Oc1cccc(C(O)CNC)c1,x
 norepinephrine|norepinephrin|noradrenaline|noradrenalin|arterenol root root
Oc1cc(C(O)CN)ccc10,x
 epinephrine|epinephrin|adrenaline|adrenalin root root Oc1cc(C(O)CNC)ccc10,x
 adrenalone root root O=C(CNC)c1ccc(O)c(O)c1,x
 norephedrine|norephedrin root root
OC(C(,x,N,n,)C),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
 ephedrine|ephedrin|pseudoephedrine|pseudoephedrin root root
OC(C(,x,N,n,C)C),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
 taurine|taurin root root C,1@x,S,x,(=O)(=O),x,C,1,C,2,N,n
 hypotaurine|hypotaurin roct root O,1@x,S,x,(=O),x,C,1,C,2,N,n
 cadaverine|cadaverin root root N,n,C,1,C,2,C,3,C,4,C,5,N,n'
 putrescine|putrescin root root N,n,C,1,C,2,C,3,C,4,N,n'
 albizzi aminoacid ine
C,1,Ring,Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,c,3|b|beta,NC(=O)N,x

alan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta
homoalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|d|delta|w
|omega
alanos aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,N,x,(,x,O,x,)
,x,N,x,=,x,O,x
alloisoleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@H],3|b|beta,(,x,
C,4|g|gamma,C,5|d|delta,),x,C,3',
allothreono|allothreon aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@H],3|b|beta,(,x,C
,4|g|gamma,),x,O,x
allys aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,=0,x
argin aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,N,nd|ndelta,C,x,(=,x,N,nw'|nomega',),x,N,nw|nomega|ngamma
asparag aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,(
=,x,O,x,),x,N,ngamma
aspart aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3,C,4|g|gamma|b|beta,(
=,x,O,x,),x,O,x
azaser aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,O,x,C(=O)C=[N
+]=[N-],x
betaalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nbeta|n3,C,2|a|alpha,C,3|b|beta,Ring,Ring1
buthion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,x,CCCC,x
canavan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,O
NC(=N)N,x
carbocyste aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s,CC(=O),x,
O,1@x
citrull aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,N,x,C,x,(=,x,O,x,),x,N,x
cycloleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,Ring,Ring2,C,3|b|beta,C,
4|g|gamma,C,5|d|delta,C,6,Ring,Ring2
cyste regineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s
cyste aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s,(=O)(=O),
x,O,1@x,
ethion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,x,C,x,C,x
isoglutam regineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,Ring,Ring2,.,x,C,2|a|alpha,Ring,Ring1,C,3|b|bet
a,C,4|g|gamma,Ring,Ring2,C,5|d|delta,(=,x,O,x,),x,N,x

glutam reqineaminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C,5|d|delta,(=,x,O,x,),x,N,nd|ndelta|n5
 glutam aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C,5|d|delta,(=,x,O,x,),x,O,1@x
 glyc aminoacid ine C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1
 histid aminoacid ine
C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,c,4,Ring,Ring2,c,5,n,1|nt|ntau|im|nim|n'|tau|prefhydro,c,2,n,3|np|npi,Ring,Ring2
 homoargin aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,N,nd|ndelta,C,x,(=,x,N,nw'|nomega'),,x,N,nw|nomega
 homocitrull aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,N,x,C,x,(=,x,O,x,),x,N,x
 homocyste reqineaminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S,s
 homocyste aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S,s,(=O)(=O),x,O,1@x
 homoglutam reqineaminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,(=,x,O,x,),x,N,ne|nepsilon|n6
 homophenylalan aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Ring,Ring2,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring2
 homoprol aminoacid ine
C,x,Ring,Ring1,,,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,C,5,C,6,Ring,Ring2
 homoser aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,O,x
 homotryptoph aminoacid ane
C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,g|gamma,C,3,Ring,Ring2,=,x,C,2,N,1,C,7a,Ring,Ring3,=,x,C,7,C,6,=,x,C,5,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
 iboten aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C2=CC(=O)NO2,x
 isoleuc aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@H],3|b|beta,(,x,C,4|g|gamma,C,5|d|delta,),x,C,3',
 isoser aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,Ring,Ring2,,x,C,2|a|alpha,Ring,Ring1,(O),x,C,3|b|beta,Ring,Ring2
 isoval aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,(,x,C,2',),x,Ring,Ring1,C,3|b|beta,C,4|g|gamma
 kynuren aminoacid ine
C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C(=O),x,c,1,Ring,Ring2,c,2,(N),x,c,3,c,4,c,5,c,6,Ring,Ring2
 leuc aminoacid ine
C1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,(,x,C,5|d|delta,),x,C,5'

lys aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,C,4|g|gamma,C
 ,5|d|delta,C,6|e|epsilon,N,n6|nw|nomega|nepsilon|ne|nz|n'
 methion aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,C,4|g|gamma,S
 ,x,C,x
 mimos aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,N2C=C(O)C(=O)
 C=C2,x
 norleuc aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,C,4|g|gamma,C
 ,5|d|delta,C,6|e|epsilon
 norval aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,C,4|g|gamma,C
 ,5|d|delta
 ornith aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,C,4|g|gamma,C
 ,5|d|delta,N,n5|ndelta|nd
 penicillam aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,(C)(C)S,x
 phenylalan|3phenylalan|betaphenylalan aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,a|alpha,Ring, Ring1,C,b|beta,c,x,Ring, Ring2,c,
 2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring, Ring2
 prol aminoacid ine
 C,x,Ring, Ring1,..,x,N,1|n|ralpha|n2,Ring, Ring2,C,2,Ring, Ring1,C,3,C,4,C,5,Ring,Ri
 ng2
 3hydroxyprol|hydroxyprol aminoacid ine
 C,x,Ring, Ring1,..,x,N,1|n|ralpha|n2,Ring, Ring2,C,2,Ring, Ring1,C,3,(O),x,C,4,C,5,R
 ing,Ring2
 4hydroxyprol aminoacid ine
 C,x,Ring, Ring1,..,x,N,1|n|ralpha|n2,Ring, Ring2,C,2,Ring, Ring1,C,3,C,4,(O),x,C,5,R
 ing,Ring2
 5hydroxyprol aminoacid ine
 C,x,Ring, Ring1,..,x,N,1|n|ralpha|n2,Ring, Ring2,C,2,Ring, Ring1,C,3,C,4,C,5,(O),x,R
 ing,Ring2
 pyroglutam aminoacid ine
 C,x,Ring, Ring1,..,x,N,1|n|ralpha|n2,Ring, Ring2,C,2,Ring, Ring1,C,3,C,4,C,5,(=O),x,
 Ring,Ring2
 sarcos aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,(,x,C,2|a|alpha,Ring, Ring1,),x,C,x
 selenocyste reqineaminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,[Se],se
 selenomethion aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,C,4|g|gamma,[
 Se],x,C,x
 ser aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,O,x
 tleuc|tertleuc aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,(,x,C,3',,)(,x
 ,C,3'',,),x,C,3''
 theano|thean aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,C,4|g|gamma,C
 ,x,(=O),x,N,x,C,x,C,x
 thiocitrull aminoacid ine
 C,1,Ring, Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring, Ring1,C,3|b|beta,C,4|g|gamma,C
 ,5|d|delta,N,x,C,x,(=,x,S,x,),x,N,x

threono|threon aminoacid ine
 C,1,Ring,Ring1,,,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@@H],3|b|beta,(,x,
 C,4|g|gamma,,),x,O,x
 tryptoph aminoacid ane
 C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,3,Ring,Ring2=,
 x,C,2,N,1,C,7a,Ring,Ring3=,x,C,7,C,6=,x,C,5,C,4=,x,C,3a,Ring,Ring2,Ring,Ring3
 thyron aminoacid ine
 C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2=,
 x,C,2|ortho,C,3|m|meta=,x,C,4,(,x,O,x,C,1',Ring,Ring3=,x,C,2',C,3'=,x,C,4',(,
 x,O,x,),x,C,5'=,x,C,6',Ring,Ring3,),x,C,5=,x,C,6,Ring,Ring2
 thyrox aminoacid ine
 C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2=,
 x,C,2|ortho,C,3|m|meta,(I),x=,x,C,4,(,x,O,x,C,1',Ring,Ring3=,x,C,2',C,3',(I),x
 ,=,x,C,4',(,x,O,x,),x,C,5',(I),x=,x,C,6',Ring,Ring3,),x,C,5,(I),x=,x,C,6,Ring,
 Ring2
 tyros|ptyros|paratyros aminoacid ine
 C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2=,
 x,C,2|ortho,C,3|m|meta=,x,C,4,(,x,O,x,),x,C,5=,x,C,6,Ring,Ring2
 mtyros|metatyros aminoacid ine
 C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2=,
 x,C,2|ortho,C,3|m|meta,(,x,O,x,),x=,x,C,4,C,5=,x,C,6,Ring,Ring2
 orthotyros aminoacid ine
 C,x,Ring,Ring1,,,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2=,
 x,C,2|ortho,(,x,O,x,),x,C,3|m|meta=,x,C,4,C,5=,x,C,6,Ring,Ring2
 val aminoacid ine
 C,1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,(,x,C,4|g|gam
 ma,),x,C,4'|5
 willardi aminoacid ine
 C,1,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,n2ccc(=O)nc(=
 O)2,x
 djenkol aminodiacid ine
 C,1,(=,x,O,x,),x,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 S,x,C,x,S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha'),,x,C,4@x=,x,O,x
 cyst aminodiacid ine
 C,1,(=,x,O,x,),x,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 S,x,S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha'),,x,C,4@x=,x,O,x
 cystathion aminodiacid ine
 C,1,(=,x,O,x,),x,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 C,4|g|gamma,S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha'),,x,C,4@x=,x,
 O,x
 homocyst aminodiacid ine
 C,1,(=,x,O,x,),x,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 C,4|g|gamma,S,x,S,x,C,4'|g'|gamma',C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|n
 pha'),,x,C,4@x=,x,O,x
 lanthion aminodiacid ine
 C,1,(=,x,O,x,),x,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha'),,x,C,4@x=,x,O,x
 selenocyst aminodiacid ine
 C,1,(=,x,O,x,),x,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 [Se],x,[Se],x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha'),,x,C,4@x=,x,O,
 x
 selenocystathion aminodiacid ine
 C,1,(=,x,O,x,),x,Ring,Ring1,,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 C,4|g|gamma,[Se],x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha'),,x,C,4@x=,
 ,x,O,x
 in|ine enderaminoacid ine O,8@x,,,x,O,5@x
 an|ane enderaminoacid ane O,8@x,,,x,O,5@x

yl enderaminoacid yl O,8@x
 ol enderaminoacid suffix O,8@x
 aceglutamide|aceglutamid root root O=C(,x,O,1@x,)C(NC(C)=O)CCC(N)=O,x
 methionol root root CSCCCO,x
 tryptophol root root
 OCC,x,c,3,Ring,Ring1,c,2,n,1,c,7a,Ring,Ring2,c,7,Ring,Ring1,c,6,c,5,c,4,c,3a,Rin
 g,Ring2

 cysteamine|cysteamin root root N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,s
 histamine|histamin root root
 N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,4,Ring,Ring2,=,x,C,5,N,1|nt|ntau,C,2,=
 ,x,N,3|np|npi,Ring,Ring2
 methioninamine|methioninamin root root
 N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,C,x
 tryptamine|tryptamin root root
 N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,7a,Ring,Rin
 g3,=,x,C,7,C,6,=,x,C,5,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
 melatonin root root
 N,n|nalpha|n2|nomega,(C(=O)C),x,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,
 7a,Ring,Ring3,=,x,C,7,C,6,=,x,C,5,(OC),x,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
 serotonin root root
 N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,7a,Ring,Rin
 g3,=,x,C,7,C,6,=,x,C,5,(O),x,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
 tyramine|tyramin|tyrosamine|tyrosamin root root
 N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,1,Ring,Ring2,=,x,C,2|ortho,C,3|m|meta,
 =,x,C,4,(,x,O,x,),x,C,5,=,x,C,6,Ring,Ring2
 cystamine|cystamin root root
 N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,S,x,C,3'|b'|beta',C,2'|a'|alpha'
 ,N,n'|na'|nalpha'
 selenocystamine|selenocystamin root root
 N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,[Se],x,[Se],x,C,3'|b'|beta',C,2'|a'|
 alpha',N,n'|na'|nalpha'
 cystathionamine|cystathionamin root root
 N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,C,3'|b'|beta',C,2'|a'|
 alpha',N,n'|na'|nalpha'
 homocystamine|homocystamin root root
 N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,S,x,C,4'|g'|gamma',C
 ,3'|b'|beta',C,2'|a'|alpha',N,n'|na'|nalpha'
 lanthionamine|lanthionamin root root
 N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,C,3'|b'|beta',C,2'|a'|alpha',N,n
 '|na'|nalpha'
 methional root root O,x,=,x,C,1,C,2,C,3,S,x,C,x

 glycero sugar hexose O,x,=,x,C,1,[C@H](,2,O,x,),x,C,3,O,x
 erythro|erythr sugar hexose
 O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,C,4,O,x
 threo|thre sugar hexose O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,C,4,O,x
 ribo|rib sugar hexose
 O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x
 arabino|arabin|arab sugar hexose
 O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x
 xylo|xyl sugar hexose
 O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x
 lyxo|lyx sugar hexose
 O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x

allo sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C, 6$
 $, O, x$
 altro|altr sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C,$
 $6, O, x$
 gluco|gluc sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C,$
 $6, O, x$
 manno|mann sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C$
 $, 6, O, x$
 gulo|gul sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C,$
 $6, O, x$
 ido sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C$
 $, 6, O, x$
 galacto|galact|dulc sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C$
 $, 6, O, x$
 talo|tal sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x,$
 $C, 6, O, x$
 boivin sugar hexose
 $O, x, =, x, C, 1, [C@H], 2, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C, 6$
 digitox sugar hexose
 $O, x, =, x, C, 1, C, 2, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C, 6$
 oli sugar hexose
 $O, x, =, x, C, 1, [C@H], 2, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C, 6$
 oliv sugar hexose
 $O, x, =, x, C, 1, [C@H], 2, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C, 6$
 glucohept sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,), x, [C@H] (, 5, O, x,) [C$
 $@H] (, 6, O, x,), x, C, 7, O, x$
 fuco|fuc sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C$
 $, 6$
 quinovo|quinov sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C,$
 6
 rhamno|rhamn sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C$
 $, 6$
 rhideo|rhode sugar hexose
 $O, x, =, x, C, 1, [C@H] (, 2, O, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C$
 $, 6$
 thymino|thymin sugar hexose
 $O, x, =, x, C, 1, [C@H], 2, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,), x, C, 5, O, x$
 galactosamine|galactosamin|chondrosamine|chondrosamin sugar trivial
 $O, x, =, x, C, 1, [C@H] (, 2, N, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C$
 $, 6, O, x$
 glucosamine|glucosamin sugar trivial
 $O, x, =, x, C, 1, [C@H] (, 2, N, x,), x, [C@H] (, 3, O, x,), x, [C@H] (, 4, O, x,) [C@H] (, 5, O, x,), x, C,$
 $6, O, x$

mannosamine|mannosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6,O,x
fucosamine|fucosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
quinovosamine|quinovosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
rhamnosamine|rhamnosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
glucal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x
rhamnal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6
galactal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x
glucamine sugar trivial
N,n,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6,O,
x
sucr sugar disugar
OC[C@H]1([C@H](O)[C@H](O)[C@H](O1)CO)O[C@H]2[C@H](O)[C@H](O)[C@H](O)[C@H](CO)
)O2,x
trehal sugar disugar
O[C@H]1[C@H](O)[C@H](CO)O[C@H](O[C@H]2[C@H](O)[C@H](O)[C@H](O)[C@H](CO)O2)[C@
H]1O,x
melezit sugar disugar
OC[C@H]1[C@H](O)[C@H](O)[C@H](O)[C@H](O[C@H]2(CO)[C@H](O[C@H]3O[C@H](CO)[C@
H](O)[C@H](O)[C@H]3O)[C@H](O)[C@H](CO)O2)O1,x
stachy|lupe sugar disugar
O[C@H]1[C@H](CO)O[C@H](OC[C@H]2O[C@H](O[C@H]3[C@H](O[C@H]4(CO)O[C@H](CO)[C@H](
O)[C@H]4O)O[C@H](CO)[C@H](O)[C@H]3O)[C@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@H]1O,
x
lact sugar disugar
OC[C@H]1O[C@H](O[C@H]([C@H](O)[C@H](O)[C@H](O)O2)[C@H]2CO)[C@H](O)[C@H](O)[
C@H]1O,x
malt|maltobi sugar disugar
O[C@H]1[C@H](O)[C@H](O[C@H]2[C@H](O)[C@H](O)[C@H](O)O[C@H]2CO)O[C@H](CO)[C@
H]1O,x
maltotri sugar disugar
O[C@H]1[C@H](O)[C@H](O)[C@H](CO)O[C@H]1O[C@H]2[C@H](CO)O[C@H](O[C@H]3[C@H]
(H)(CO)OC(O)[C@H](O)[C@H]3O)[C@H](O)[C@H]2O,x
maltotetra sugar disugar
O[C@H]([C@H](O[C@H]4[C@H](O)[C@H]([C@H](O)O[C@H]4CO)O)O[C@H]1CO)[C@H](O)[C@
H]1O[C@H]2[C@H](O)[C@H]([C@H](O[C@H](O[C@H](CO)[C@H]3O)[C@H](O)[C@H]3O)[C@H]
](CO)O2)O,x
maltopenta sugar disugar
O[C@H]([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@H]1[C@H](CO)O[C@H](O[C@H]3[C@H](O)[
C@H]([C@H](O[C@H]4[C@H](O)[C@H]([C@H](O[C@H]5[C@H](O)[C@H]([C@H](O)O[C@H]5CO
)O)O[C@H]4CO)O)O[C@H]3CO)O)[C@H](O)[C@H]1O,x
maltohexa sugar disugar
O[C@H]([C@H](O[C@H]3[C@H](O)[C@H]([C@H](O[C@H]6[C@H](O)[C@H]([C@H](O)O[C@H]
6CO)O)O[C@H]3CO)O)O[C@H]1CO)[C@H](O)[C@H]1O[C@H]2[C@H](O)[C@H]([C@H](O[C@H]
]4[C@H](O)[C@H]([C@H](O[C@H](O[C@H](CO)[C@H]5O)[C@H](O)[C@H]5O)[C@H](CO)O4)O)[
C@H](CO)O2)O,x

melibi sugar disugar
O[C@H]1[C@@H](OC[C@H]([C@H](O)[C@H](O)[C@H]2O)O[C@H]2O)O[C@H](CO)[C@H](O)[C@H]1O,x
 cellobi sugar disugar
OC[C@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@H](O[C@H]2[C@@H](CO)O[C@H](O)[C@H](O)[C@H]2O)O1,x
 cellotri sugar disugar
O[C@H]([C@H]1O)[C@H](O[C@H]2[C@@H](O)[C@H]([C@H](O[C@H]3[C@H](O)[C@H](C(O)O[C@H]3CO)O[C@H]2CO)O)[C@H](CO)[C@H]1O,x
 cellotetra sugar disugar
OC(O[C@H](CO)[C@H]1O[C@H]2[C@@H](O)[C@H](O)[C@H](O[C@H]3[C@H](O)[C@H](O[C@H]4[C@H](O)[C@H](O)[C@H](CO)O4)[C@H](CO)O3)[C@H](CO)O2)[C@H](O)[C@H]1O,x
 cellopenta sugar disugar
OC(O[C@H]1CO)[C@H](O)[C@@H]([C@H]1O[C@H]2[C@@H](O)[C@H](O)[C@H](O[C@H]3O[C@H]4[C@H](O)[C@H](O)[C@H](O[C@H]5[C@H](O)[C@H](O)[C@H](O)[C@H](CO)O5)[C@H](CO)O4)[C@H](O)[C@H]3O)[C@H](CO)O2)O,x
 chitobi sugar disugar
N,n,[C@H]([C@H](O)O[C@H]2CO)[C@H](O)[C@H]2O[C@H](O1)[C@H](,x,N,n',)[C@H](O)[C@H](O)[C@H]1CO,x
 chitotri sugar disugar
N,n,[C@H](C(O)O[C@H]3CO)[C@H](O)[C@H]3O[C@H](O[C@H]1CO)[C@H](,x,N,n',)[C@H](O)[C@H]1O[C@H](O[C@H](CO)[C@H]2O)[C@H](,x,N,n',)[C@H]2O,x
 raffin|melit|meli tri sugar disugar
OC[C@H]1OC(OC[C@H]2OC(O[C@H]3(CO)[C@H](O)[C@H](O)[C@H](CO)O3)[C@H](O)[C@H]2O)[C@H](O)[C@H]1O,x
 gentiobi sugar disugar
O[C@H]1[C@H](OC[C@H](O)[C@H](O)[C@H]2O)O[C@H]2O)O[C@H](CO)[C@H](O)[C@H]1O,x
 palatin sugar disugar
OC[C@H]1(O)O[C@H](CO[C@H]2[C@H](O)[C@H](O)[C@H](O)[C@H](CO)O2)[C@H](O)[C@H]1O,x
 turan sugar disugar
O[C@H]([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@H]1C(O)(CO)OC[C@H](O)[C@H]1O,x
 ose endersugar ose x,x
 itol endersugar itol x,x
 ityl endersugar makefree x,x
 ide|id|oside|osid endersugar oside x,x
 on|ono endersugar on x,x
 uron|uron endersugar uron x,x
 ar|aro endersugar ar x,x
 odialdo|odiald endersugar dialdo x,x
 oxirose|oxiros pyranose unknown 2,x
 oxetose|oxetos pyranose unknown 3,x
 furanose|furanos|ofuranose|ofuranos pyranose unknown 4,x
 pyranose|pyranos|opyranose|opyranos pyranose unknown 5,x
 septanose|septanos|oseptanose|oseptanos pyranose unknown 6,x
 tetro multisugar unknown 4,x
 pento multisugar unknown 5,x
 hexo multisugar unknown 6,x
 hepto multisugar unknown 7,x
 octo multisugar unknown 8,x
 nono multisugar unknown 9,x
 deco multisugar unknown 10,x
 ulo|ul structsgarender ulose C=O,x
 osamine structsgarender osamine N,x
 deoxy|desoxy deoxy unknown C,x

inositol pseudosugar unknown x,x
 inositol root root OC1C(O)C(O)C(O)C(O)C1O,x
 mesoinositol|myoinositol root root
 O,x,[C@H],1,Ring,Ring1,[C@H],2,(O),x,[C@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O),
 x,[C@H],6,Ring,Ring1,O,x
 scylloinositol root root
 O,x,[C@H],1,Ring,Ring1,[C@H],2,(O),x,[C@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O),x
 ,,[C@H],6,Ring,Ring1,O,x
 epiinositol root root
 O,x,[C@H],1,Ring,Ring1,[C@H],2,(O),x,[C@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O)
 ,x,[C@H],6,Ring,Ring1,O,x
 dinositol root root O[C@H]1[C@H](O)[C@H](O)[C@H](O)[C@H]1O,x
 linositol root root O[C@H]1[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H]1O,x
 quebrachitol root root O[C@H]1[C@H](O)[C@H](O)[C@H](O)(OC)[C@H](O)[C@H]1O,x
 muram pseudosugar unknown x,x
 muram root root
 CC(C)O,x,[C@H],3,Ring,Ring1,[C@H],4,(O),x,[C@H],5,(,x,C,6,O,x,),x,O,x,[C@H],1,(
 O),x,[C@H],2,(,x,N,n,),x,Ring,Ring1
 neuramin pseudosugar unknown x,x
 neuramin root root
 C,x,[C@H],2,Ring,Ring1,(O),x,O,x,[C@H],6,(,x,[C@H],7,(O),x,[C@H],8,(O),x,C,9,O,
 x,),x,[C@H],5,(,x,N,n,),x,[C@H],4,(O),x,C,3,Ring,Ring1
 sial pseudosugar unknown x,x
 sial root root
 C,x,[C@H],2,Ring,Ring1,(O),x,O,x,[C@H],6,(,x,[C@H],7,(O),x,[C@H],8,(O),x,C,9,O,
 x,),x,[C@H],5,(,x,NC(=O)C,x,),x,[C@H],4,(O),x,C,3,Ring,Ring1

 adenos|adenyl nucleotide nucleotide
 O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Rin
 g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(,x,N,n|n6,),x,n,1,c,2,n,3
 ,c,4,Ring,Ring3,Ring,Ring2
 cytid|cytidyl nucleotide nucleotide
 O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Rin
 g,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3,c,4,(,x,N,n|n4,),x,c,5,c,6,Ring,Ring2
 guanos|guanyl nucleotide nucleotide
 O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Rin
 g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(=O),x,N,1,c,2,(,x,N,n|n2,
),x,n,3,c,4,Ring,Ring3,Ring,Ring2
 inos nucleotide nucleotide
 O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Rin
 g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(O),x,n,1,c,2,n,3,c,4,Ring
 ,Ring3,Ring,Ring2
 thymid|thymidyl nucleotide nucleotide
 O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,C,2',[C@H],1',(O,x,Ring,Ring1,),x
 ,n,1,Ring,Ring2,c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,(C),x,c,6,Ring,Ring2
 urid|uridyl nucleotide nucleotide
 O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Rin
 g,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,c,6,Ring,Ring2
 xanthos|xanthoyl|xanthonyl nucleotide nucleotide
 O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Rin
 g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(O),x,n,1,c,2,(O),x,n,3,c,
 4,Ring,Ring3,Ring,Ring2
 orotid|orotidyl nucleotide nucleotide
 O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Rin
 g,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3,c,4,(=O),x,c,5,c,6,(C(=O)O),x,Ring,Rin
 g2

cordycep nucleotide nucleotide
O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',[C@H],2',(O),x,[C@H],1',(O,x,Ring,Ring1,,x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(x,N,n|n6,),x,n,1,c,2,n,3,c,4,Ring,Ring3,Ring,Ring2
 adenyl loveracid root
P,x,(=O),x,(x,O,1@o,),x,(x,O,1@o,),x,O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(x,N,n|n6,),x,n,1,c,2,n,3,c,4,Ring,Ring3,Ring,Ring2
 cytidyl loveracid root
P,x,(=O),x,(x,O,1@o,),x,(x,O,1@o,),x,O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Ring,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3,c,4,(x,N,n,),x,c,5,c,6,Ring,Ring2
 guanyl loveracid root
P,x,(=O),x,(x,O,1@o,),x,(x,O,1@o,),x,O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(=O),x,n,1,c,2,(x,N,n|n2,)n,3,c,4,Ring,Ring3,Ring,Ring2
 inos loveracid root
P,x,(=O),x,(x,O,1@o,),x,(x,O,1@o,),x,O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(O),x,n,1,c,2,n,3,c,4,Ring,Ring3,Ring,Ring2
 thymidyl loveracid root
P,x,(=O),x,(x,O,1@o,),x,(x,O,1@o,),x,O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,C,2',[C@H],1',(O,x,Ring,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,(C),x,c,6,Ring,Ring2
 uridylyl loveracid root
P,x,(=O),x,(x,O,1@o,),x,(x,O,1@o,),x,O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Ring,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,c,6,Ring,Ring2
 xanthoyl|xanthonyl loveracid root
P,x,(=O),x,(x,O,1@o,),x,(x,O,1@o,),x,O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(O),x,n,1,c,2,(O),x,n,3,c,4,Ring,Ring3,Ring,Ring2
 purineriboside root root
O,x,C,5',[C@H],4',Ring,Ring1,[C@H],3',(O),x,[C@H],2',(O),x,[C@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,n,1,c,2,n,3,c,4,Ring,Ring3,Ring,Ring2
 thuj root root
C,3,Ring,Ring1,C,2,C,1,Ring,Ring2,(x,C,7,(x,C,8,),x,C,9,),x,C,6,C,5,Ring,Ring2,C,4,Ring,Ring1,(x,C,10,),x
 car root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,(x,C,4,C,5,C,6,Ring,Ring1,(x,C,7,Ring,Ring2,(x,C,8,),x,C,9,),x,C,10
 norcar root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,C,5,C,6,Ring,Ring1,(x,C,7,Ring,Ring2,),x
 pin root root
C,2,Ring,Ring1,(x,C,10,),x,C,3,C,4,C,5,(x,C,7,Ring,Ring2,),x,C,6,(x,C,8,)(x,C,9,),x,C,1,Ring,Ring2,Ring,Ring1
 norpin root root
C,2,Ring,Ring1,C,3,C,4,C,5,(x,C,7,Ring,Ring2,),x,C,6,C,1,Ring,Ring2,Ring,Ring1
 camphor loveracid root
C,10,C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(x,C,5,C,6,Ring,Ring1,),x,C,7,(x,C,8,),x,(x,C,9,),x,Ring,Ring2
 camphor root root
C,10,C,1,Ring,Ring1,Ring,Ring2,C,2,(=O),x,C,3,C,4,(x,C,5,C,6,Ring,Ring1,),x,C,7,(x,C,8,),x,(x,C,9,),x,Ring,Ring2

norcamphor root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,(=O),x,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,Ring
 ,Ring2
 camphorquinone|camphoroquinone root root
 C,10,C,1,Ring,Ring1,Ring,Ring2,C,2,(=O),x,C,3,(=O),x,C,4,(,x,C,5,C,6,Ring,Ring1,
),x,C,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
 borne|born|camphane|camphan|bornylane|bornylan|isoborne|isoborn root root
 C,2,Ring,Ring1,C,3,C,4,Ring,Ring2,C,5,C,6,C,1,Ring,Ring1,(,x,C,7,Ring,Ring2,(,x,
 C,8,),x,C,9,),x,C,10
 camphan loveracid root
 C,1,Ring,Ring1,Ring,Ring2,O,2,C,3,(=O),x,C,4,(,x,C,5,C,6,Ring,Ring1,),x,(,x,C,7,
 (,x,C,x,)(,x,C,x,),x,Ring,Ring2,),x,C,x
 norborne|norborn|norborna root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,Ring,Ring2
 norbornadien|norbornadiene|25norbornadien|25norbornadiene root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,=,x,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,C,7,Rin
 g,Ring2
 norbornen|norbornene|2norbornen|2norbornene root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,C,7,Ring,Ri
 ng2
 5norbornen|5norbornene root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,C,7,Ring,Ri
 ng2
 camphene|camphen root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,(,x,C,x,),x,(,x,C,x,),x,C,3,(,x,=,x,C,x,),x,C,4,(,
 x,C,5,C,6,Ring,Ring1,),x,C,7,Ring,Ring2
 phosgene|phosgen root root ClC(=O)Cl,x
 triphosgene|triphosgen root root C(C1)(C1)(C1)OC(=O)OC(C1)(C1)(C1),x
 glyoxyl root root C,1,C,2|w|omega,=,x,O,x
 pyruv root root C,1,C,2,(=,x,O,x,),x,C,3|w|omega
 glycerol|snglycerol|racglycerol pseudosugar unknown x,x
 glycerol|snglycerol|snglycero|racglycerol|racglycero|glycerine root root
 O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma
 glycerin root root O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma
 glycerone|glyceron root root O,1@1|a|alpha,C,x,C,x,(=O),x,C,x,O,1@3|g|gamma
 in|anooin glycerin root
 O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma|a'|alpha'
 gerani|geran root root
 C,1,/,x,C,2,=,x,C,3,(,x,C,x,),x,/,x,C,4,C,5,C,6,=,x,C,7,(,x,C,x,),x,C,8
 tetrahydrogerani|geran root root
 C,1,C,2,C,3,(,x,C,x,),x,C,4,C,5,C,6,C,7,(,x,C,x,),x,C,8
 ner root root
 C,1,/,x,C,2,=,x,C,3,(,x,C,x,),x,\,x,C,4,C,5,C,6,=,x,C,7,(,x,C,x,),x,C,8
 phyt root root
 C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,(,x,C,x,),x,
 C,x,C,x,C,x,(,x,C,x,),x,C,x
 citral root root
 O,x,=,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x
 ethylcitral root root
 O,x,=,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x
 citronell|betacitronell|baran root root CCC(C)CCC=C(C)C,C,x
 linalo root root C(CCC=C(C)C)(C=C)C,x
 dihydrolinalo root root C(CCC=C(C)C)(CC)C,x
 tetrahydrolinalo root root C(CCCC(C)C)(CC)C,x
 lavandul root root CC(C(=C)C)CC=C(C)C,x
 tetrahydrolavandul root root CC(C(C)C)CCC(C)C,x

farnes root root
 C,1,C,2,=,x,C,3,(C),x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8,C,9,C,10,=,x,C,11,(C)C,x
 ocimene root root C,1,=,x,C,2,C,3,(C)=,x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8
 alloocimene|allocimen root root
 C,1,C,2,(C)=,x,C,3,C,4,=,x,C,5,(C),x,C,6,=,x,C,7,C,8
 nerolid root root C(C)(C=C)CCC=C(C)CCC=C(C)C,x
 all root root C,1|a|alpha,C,2|b|beta,=,x,C,3|g|gamma
 isoall root root C,1|a|alpha,=,x,C,2|b|beta,C,3|g|gamma
 homoall root root C,1|a|alpha,C,2|b|beta,C,3|g|gamma,=,x,C,4|d|delta
 methall root root C,1,C,2,(,x,C,x,),x,=,x,C,3
 triazeno root root N,4@1,=,x,N,2,N,3
 vin root root C,1|a|alpha,=,x,C,2|b|beta
 hydrazine|hydrazin root root N,1|n,N,2|n'
 dithioiminocarbonate root root S,1@s,C,x,(=,x,N,n,),x,S,1@s'
 urea|carbamide|carbamid root root N,1|n,C,2,(,x,=,x,O,o,),x,N,3|n'
 sulfocarbamide|sulfocarbamid|sulfourea root root
 N,1|n,C,2,(,x,=,x,S,s,),x,N,3|n'
 biurea root root N,1,C,2,(=O),x,N,3,N,4,C,5,(=O),x,N,6
 guanyl root root C,4@x,(=N),x,N,x
 uronium root root N,1|n,C,2,(,x,N,3|n'),,x,=,x,[O+],o
 ureido root root N,4@1|n,C,2,(,x,=,x,O,o,),x,N,3|n'
 ureylene|ureylen root bridge N,4@1|n,C,2,(,x,=,x,O,o,),x,N,4@3|n'
 carbanilide|carbanilid root root
 c,6,Ring,Ring1,c,5,c,4,c,3,c,2,c,1,Ring,Ring1,N,n,C,x,(,x,=,x,O,o,),x,N,n',c,1',
 Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
 tms root root [Si],4@x,(C)(C)(C),x
 tbdms root root [Si],4@x,(C(C)(C)C)(C)(C),x
 plumb root root [Pb],1
 sil root root [Si],x
 stann root root [Sn],x
 bor root root [B],x
 germ root root [Ge],x
 amine|amin|ammonia root root N,n
 phosphine|phosphin root root P,x
 arsine|arsin root root [As],x
 hydrogen root root [H],4@x
 deuterium root root [2H],4@x
 tritium root root [3H],4@x
 hydrido root root [H-],4@x
 deuterido root root [2H-],4@x
 lithio root root [Li],4@x
 sodio root root [Na],4@x
 potassio|kalio root root [K],4@x
 fluoro|fluor root root F,4@x
 chloro|chlor root root Cl,4@x
 chlorosyl root root Cl,4@x,=O,x
 chloryl root root Cl,4@x,(=O)=O,x
 perchloryl root root Cl,4@x,(=O)(=O)=O,x
 borono root root [B],4@x,(O)O,x
 lithium root metal [Li],x
 sodium|natrimum root metal [Na],x
 potassium|kalium root metal [K],x
 rubidium root metal [Rb],x
 cesium root metal [Cs],x
 francium root metal [Fr],x
 beryllium|glucinium root metal [Be],x
 magnesium root metal [Mg],x

calcium root metal [Ca],x
strontium root metal [Sr],x
barium root metal [Ba],x
radium root metal [Ra],x
scandium root metal [Sc],x
yttrium root metal [Y],x
lanthanum root metal [La],x
cerium root metal [Ce],x
praesodymium|praseodymium root metal [Pr],x
neodymium root metal [Nd],x
promethium root metal [Pm],x
samarium root metal [Sm],x
europium root metal [Eu],x
gadolinium root metal [Gd],x
terbium root metal [Tb],x
dysprosium root metal [Dy],x
holmium root metal [Ho],x
erbium root metal [Er],x
thulium root metal [Tm],x
ytterbium root metal [Yb],x
lutetium|cassiopeium root metal [Lu],x
actinium root metal [Ac],x
thorium root metal [Th],x
protactinium root metal [Pa],x
uranium root metal [U],x
neptunium root metal [Np],x
plutonium root metal [Pu],x
americium root metal [Am],x
curium root metal [Cm],x
berkelium root metal [Bk],x
californium root metal [Cf],x
einsteinium root metal [Es],x
fermium root metal [Fm],x
mendelevium root metal [Md],x
nobelium root metal [No],x
lawrencium root metal [Lr],x
titanium root metal [Ti],x
zirconium root metal [Zr],x
hafnium root metal [Hf],x
vanadium root metal [V],x
niobium root metal [Nb],x
tantalum root metal [Ta],x
chromium root metal [Cr],x
molybdenum root metal [Mo],x
tungsten root metal [W],x
manganese root metal [Mn],x
technetium root metal [Tc],x
rhenium root metal [Re],x
iron root metal [Fe],x
ruthenium root metal [Ru],x
osmium root metal [Os],x
cobalt root metal [Co],x
rhodium root metal [Rh],x
iridium root metal [Ir],x
nickel root metal [Ni],x
palladium root metal [Pd],x
platinum root metal [Pt],x

copper root metal [Cu],x
silver|argent root metal [Ag],x
gold root metal [Au],x
zinc root metal [Zn],x
cadmium root metal [Cd],x
mercury root metal [Hg],w
boron root nonmetal [B],x
aluminum|alane root metal [Al],x
gallium root metal [Ga],x
indium root metal [In],x
thallium root metal [Tl],x
carbon root nonmetal [C],x
silicon root nonmetal [Si],x
germanium root metal [Ge],x
tin root metal [Sn],x
lead root metal [Pb],x
nitrogen root nonmetal [N],x
phosphorus root nonmetal [P],x
arsenic root nonmetal [As],x
antimony|stibium root metal [Sb],x
bismuth root metal [Bi],x
oxygen root nonmetal [O],x
sulfur root nonmetal [S],x
selenium root nonmetal [Se],x
tellurium root nonmetal [Te],x
polonium nonroot metal [Po],x
fluorine root nonmetal [F],x
chlorine root nonmetal [Cl],x
bromine root nonmetal [Br],x
iodine root nonmetal [I],x
astatine root nonmetal [At],x
helium root nonmetal [He],x
neon root nonmetal [Ne],x
argon root nonmetal [Ar],x
krypton root nonmetal [Kr],x
xenon root nonmetal [Xe],x
radon root nonmetal [Rn],x

bromo|brom root root Br,4@x
iodo|iod root root I,4@x
iodosyl|iodoso root root I,4@x,=O,x
iodyl|iodoxy root root I,4@x,(=O)=O,x
deutero|deuterio root root [2H],4@x
nitro root root [N+],4@x,(=O)[O-],x
acinitro root root [N+],8@x,(O)[O-],x
nitroso|nitros|nitrosyl root root N=O,4@x
nitrosamido root root N,4@x,N=O,x
nitrosamide root root NN=O,x
nitrosonium root root [NH0+],x,=O,x
isonitroso|isonitros root root N,8@x,O,x
hydroxy|hydroxo root root O,4@x
hydroxyl root root O,4@o
hydroseleno root root [Se],4@x
hydrotelluro root root [Te],4@x
cyano|cyanogen root root C#N,4@x
isocyano|isonitrilo root root [N+]#[C-],4@x
cyanato root root OC#N,4@x

isocyanato root root N=C=O, 4@x
 thiocyanato root root SC#N, 4@x
 isothiocyanato root root N=C=S, 4@x
 selenocyanato root root [Se]C#N, 4@x
 isoselenocyanato root root N=C=[Se], 4@x
 diazo root root [N+], 8@x, =[N-], x
 diazoate|diazoat root root [N+], 8@x, =N, x, [O-], x
 azido|triazo root root N, 4@x, =[N+]=[N-], x
 oxo|keto root root O, 8@x
 oxido root root [O-], 4@x
 thioxo|thiono root root S, 8@x
 sulfido root root [S-], 4@x
 selenoxo root root [Se], 8@x
 telluroxo root root [Te], 8@x
 mercapto root root S, 4@x
 hydroperoxy root root O, 4@x, O, x
 carboxy root root C, 4@x, (=, x, O, x,), x, O, x
 amidino root root C, 4@x, (, x, N, x,)=, x, N, x
 aminoiminometh root root C, x, (=, x, N, x,), x, N, x
 sulfo root heterolover S, 4@x, (=O), x, (=O), x, O, x
 sulfoxy root root O, 4@x, S, x, (=O), x, (=O), x, O, x
 sulfoamido root root N, 4@x, S, x, (=O), x, (=O), x, O, x
 sulfino root root S, 4@x, (=O), x, O, x
 sulfeno root root S, 4@x, O, x
 sulfonato root root S, 4@x, (=O), x, (=O), x, [O-], x
 phosphonato|phosphato root root P, 4@x, (=O), x, ([O-]), x, [O-], x
 hydrogenphosphato root root P, 4@x, (=O), x, (O), x, [O-], x
 dihydrogenphosphato root root P, 4@x, (=O), x, (O), x, O, x
 phosphinato root root P, 4@x, (=O), x, [O-], x
 phosphono|phosphoro infix infix P, 4@x, (=O), x, (, x, O, 1@o',), x, O, 1@o
 phospho root heterolover P, 4@x, (=O), x, (O), 1@x, O, 1@x
 diphospho root heterolover P, 4@x, (=O), x, (O), 1@x, O, x, P, x, (=O), x, (O), 1@x, O, 1@x
 triphospho root heterolover
 P, 4@x, (=O), x, (O), 1@x, O, x, P, x, (=O), x, (O), 1@x, O, 1@x
 phosphinico root root P, 8@x, (=O), x, O, 1@o
 arsonato root root [As], 4@x, (=O), x, ([O-]), x, [O-], x
 arsinato root root [As], 4@x, (=O), x, [O-], x
 arsono|arsoro root root [As], 4@x, (=O), x, (, x, O, 1@o',), x, O, 1@o
 arsinico root root [As], 8@x, (=O), x, O, 1@o
 mesyl root root S, 4@x, (=O), x, C, x
 -part2-toluene root root C, 4@a|alpha
 -part2-cumene root root C, 4@7|a|alpha, (, x, C, 8|b|beta,), x, C, 9
 -part2-cymene root root C, 4@8|a|alpha, (, x, C, 9,), x, C, 10
 -part2-anisidine root root O, 4@x, C, a|alpha
 -part2-thioanisidine root root S, 4@x, C, a|alpha
 -part2-phenetidine root root O, 4@x, C, a|alpha, C, b|beta
 -part2-xylidine root root C, 4@a|alpha
 -part2-arsanil root root N, 4@n
 -part2-coumar root root O, 4@x
 indophenol root root
 O, x, =, x, C, 1, Ring, Ring1, C, 2, =, x, C, 3, C, 4, (, x, C, 5, =, x, C, 6, Ring, Ring1,), x, =, x, N, x, C,
 1', Ring, Ring2, =, x, C, 2' |m|meta, C, 3' |o|ortho, =, x, C, 4', (, x, O, x,), x, C, 5', =, x, C, 6', Ri
 ng, Ring2
 thymolindophenol root root
 O, x, =, x, C, 1, Ring, Ring1, C, 2, =, x, C, 3, C, 4, (, x, C, 5, =, x, C, 6, Ring, Ring1,), x, =, x, N, x, C,
 1', Ring, Ring2, =, x, C, 2' |m|meta, C, 3' |o|ortho, (, x, C, x, (, x, C, x,), x, C, x,), x, =, x, C, 4',
 (, x, O, x,), x, C, 5', =, x, C, 6', (, x, C, x,), x, Ring, Ring2

cresolindophenol root root
 $O, x, =, x, C, 1, \text{Ring}, \text{Ring}1, C, 2, =, x, C, 3, C, 4, (, x, C, 5, =, x, C, 6, \text{Ring}, \text{Ring}1,), x, =, x, N, x, C, 1', \text{Ring}, \text{Ring}2, =, x, C, 2' | m | \text{meta}, (C), x, C, 3' | o | \text{ortho}, =, x, C, 4', (, x, O, x,), x, C, 5', =, x, C, 6', \text{Ring}, \text{Ring}2$
 picoline|picolin|picol toluene picoline
 $c, 2, \text{Ring}, \text{Ring}1, c, 3 | b | \text{beta}, c, 4 | g | \text{gamma}, c, 5, c, 6, n, 1, \text{Ring}, \text{Ring}1$
 pipecoline|pipecolin|pipecol toluene picoline
 $C, 2 | a | \text{alpha}, \text{Ring}, \text{Ring}1, C, 3 | b | \text{beta}, C, 4 | g | \text{gamma} | p, C, 5, C, 6, N, 1, \text{Ring}, \text{Ring}1$
 toluene|tolu|tol toluene toluene
 $c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, \text{Ring}, \text{Ring}2, ., x, c, 4 | p | \text{para}, \text{Ring}, \text{Ring}3, \text{Ring}, \text{Ring}4, ., x, c, 6, \text{Ring}, \text{Ring}5, \text{Ring}, \text{Ring}1, ., x, c, 3 | m | \text{meta}, \text{Ring}, \text{Ring}2, \text{Ring}, \text{Ring}3, ., x, c, 5, \text{Ring}, \text{Ring}4, \text{Ring}, \text{Ring}5$
 toluidide|toluidide|toluidide toluidide toluene
 $O, 8 @ x, ., x, N, 4 @ x, c, 1', \text{Ring}, \text{Ring}1, c, 2' | o | \text{ortho}, c, 3' | m | \text{meta}, c, 4' | p | \text{para}, c, 5', c, 6', \text{Ring}, \text{Ring}1$
 cumidine|cumidin toluene cumene
 $N, n, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, =, x, c, 6, \text{Ring}, \text{Ring}1$
 cumene|cumen toluene cumene
 $c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, =, x, c, 6, \text{Ring}, \text{Ring}1$
 cumyl|alphacumyl root root
 $C, 4 @ a | \text{alpha}, (C) (C), x, c, 1, \text{Ring}, \text{Ring}1, c, 2, c, 3, c, 4, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 cumidene|cumiden toluene cumene
 $N, n, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, =, x, c, 6, \text{Ring}, \text{Ring}1$
 cymene|cymen toluene cymene
 $C, 7 | a | \text{alpha}, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 xylene|xylol toluene toluene
 $C, a | \text{alpha}, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 xylen|xyl toluene xylidine
 $c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 xylidine|oxylidide|xylide|oxylide toluidide xylidine
 $O, 8 @ x, ., x, N, 4 @ x, c, 1', \text{Ring}, \text{Ring}1, c, 2' | o | \text{ortho}, c, 3' | m | \text{meta}, c, 4' | p | \text{para}, c, 5', c, 6', \text{Ring}, \text{Ring}1$
 anis toluene anisidine
 $c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 thioanis toluene thioanisidine
 $c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 homoanis toluene anisidine
 $C, x, C, x, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 anisidide|oanisidide|aniside|oaniside toluidide anisidine
 $O, 8 @ x, ., x, N, 4 @ x, c, 1', \text{Ring}, \text{Ring}1, c, 2' | o | \text{ortho}, c, 3' | m | \text{meta}, c, 4' | p | \text{para}, c, 5', c, 6', \text{Ring}, \text{Ring}1$
 anisal toluene anisidine
 $C, 8 @ x, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 mentha|menth|neomenth|neomentha|isomenth|isomentha toluene cymene
 $c, 3 | m | \text{meta}, \text{Ring}, \text{Ring}1, C, 4 | p | \text{para}, c, 5, c, 6, C, 1, \text{Ring}, \text{Ring}2, C, 2 | o | \text{ortho}, \text{Ring}, \text{Ring}1, ., x, C, 7 | a | \text{alpha}, \text{Ring}, \text{Ring}2$
 anisidine|anisidin toluene anisidine
 $N, n, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 anisidino toluene anisidine
 $N, 4 @ n, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 phenetidine|phenetidin toluene phenetidine
 $N, n, c, 1, \text{Ring}, \text{Ring}1, c, 2 | o | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 phenetidide|ophenetidide|phenetide|ophenetide toluidide phenetidine
 $O, 8 @ x, ., x, N, 4 @ x, c, 1', \text{Ring}, \text{Ring}1, c, 2' | o | \text{ortho}, c, 3' | m | \text{meta}, c, 4' | p | \text{para}, c, 5', c, 6', \text{Ring}, \text{Ring}1$
 phenetidino toluene phenetidine
 $N, 4 @ n, c, 1, \text{Ring}, \text{Ring}1, c, 2 | c | \text{ortho}, c, 3 | m | \text{meta}, c, 4 | p | \text{para}, c, 5, c, 6, \text{Ring}, \text{Ring}1$

cresyl toluene toluene
 O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
 cres toluene toluene
 c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 thiocresol toluene toluene
 S,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 cresylicacid toluene toluene
 O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 cresot toluene toluene
 c,2,Ring,Ring1,(O),x,c,3|o|ortho,c,4|m|meta,c,5|p|para,c,6,c,1,(,x,C,x,),x,Ring,
 Ring1
 toluidine|toluidin toluene toluene
 N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 toluidino toluene toluene
 N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 xylidine|xylidin toluene xylidine
 N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 xylidino toluene xylidine
 N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 coumar toluene coumar
 C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
 c,6,Ring,Ring1
 arsanil toluene tolarsanil
 [As],x,(,x,O,1@x,),x,(,x,O,1@x,),x,(=O),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,
 c,4|p|para,c,5,c,6,Ring,Ring1
 tosyl|ptosyl root root
 S,4@x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc,x,(,x,C,x,),x,cc,x,Ring,Ring1
 tosylate|ptosylate|tosylat|ptosylat|tosilate|ptosilate|tosilat|ptosilat root
 root O,1@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(C)cc,x,Ring,Ring1
 tosylamido root root
 N,4@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(C)cc,x,Ring,Ring1
 brosylate|brosylat|brosilate|brosilat root root
 O,1@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(Br)cc,x,Ring,Ring1
 brosyl root root S,4@x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(Br)cc,x,Ring,Ring1
 closylate|closylat|closilate|closilat root root
 O,1@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(Cl)cc,x,Ring,Ring1
 closyl root root S,4@x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(Cl)cc,x,Ring,Ring1
 nosylate|nosylat|nosilate|nosilat root root
 O,1@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,cc([N+] (=O) [O-])ccc,x,Ring,Ring1
 mesylate|mesylat root root O,1@x,S,x,(=O),x,(=O),x,C,x
 esylate|esylat root root O,1@x,S,x,(=O),x,(=O),x,C,x,C,x
 pipsyl root root S,4@x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(I)cc,x,Ring,Ring1
 methosulfate|methosulfat|metilsulfate|metilsulfat root root
 O,1@x,S,x,(=O),x,(=O),x,O,x,C,x
 ethosulfate|ethosulfat|etilsulfate|etilsulfat root root
 O,1@x,S,x,(=O),x,(=O),x,O,x,C,x,C,x
 desyl root root C,x,(C(=O)c1cccc1)c2cccc2,x
 isoniazide|isoniazid root root
 c,2,Ring,Ring1,c,3,c,4,(,x,C,x,(,x,=,x,O,x,),x,N,x,N,n,),x,c,5,c,6,n,1,Ring,Ring
 1
 pheneth root root
 C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring
 ,Ring1
 secpheneth root root
 C,a|alpha,(,x,C,b|beta,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
 c,6,Ring,Ring1

neoph root root
 C,a|alpha,C,b|beta,(C)(C),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5
 ,c,6,Ring,Ring1
 amphetamine|amphetamin root root
 N,n,C,a|alpha,(C),x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,
 5,c,6,Ring,Ring1
 methamphetamine|methamphetamine root root
 C,x,N,n,C,a|alpha,(C),x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|par
 a,c,5,c,6,Ring,Ring1
 ammeline root root
 N,n,c,6,Ring,Ring1,n,1,c,2,(,x,0,x,),x,n,3,c,4,(,x,0,x,),x,n,5,Ring,Ring1
 phenate|phenat|phenoxyde|phenoxyd root root [O-
],x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 phen root phenyl
 c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 benzyne|benzyn root root
 C,1,Ring,Ring1,#,x,C,2|o|ortho,C,3|m|meta,=,x,C,4|p|para,C,5,=,x,C,6,Ring,Ring1
 benzal root root
 C,8@a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 benzene|benzen|benzol root root
 c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 dewarbenzene root root C12C=CC1C=C2,x
 benzeneoxid|benzeneoxide root root
 C,1,Ring,Ring1,(,x,0,x,Ring,Ring2,),x,C,2,Ring,Ring2,C,3,=,x,C,4,C,5,=,x,C,6,Rin
 g,Ring1
 benzo-quinone|benzo-quinon root root
 C,1,Ring,Ring1,(=O),x,C,2|o|ortho,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x,C,6,R
 ing,Ring1
 benzo-quinodimethane|benzo-quinodimethan root root
 C,1,Ring,Ring1,(=,x,C,2@7,),x,C,2|o|ortho,=,x,C,3|m|meta,C,4|p|para,(=,x,C,2@8,)
 ,x,C,5,=,x,C,6,Ring,Ring1
 toluquinone|ptoluquinone root root
 C,1,Ring,Ring1,(=O),x,C,2|o|ortho,(C),x,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x
 ,C,6,Ring,Ring1
 xyloquinone|pxyloquinone root root
 C,1,Ring,Ring1,(=O),x,C,2|o|ortho,(C),x,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x
 ,C,6,(C),x,Ring,Ring1
 duroquinone root root CC(C(C(C)=C1C)=O)=C(C1=O)C,x
 thymoquinone root root O=C(C(C)=C1)C=C(C1=O)C(C)C,x
 hemellitol root root
 c,1,(C),x,Ring,Ring1,c,2|o|ortho,(C),x,c,3|m|meta,(C),x,c,4|p|para,c,5,c,6,Ring,
 Ring1
 benzo|benz benz benzo
 c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 acene|acen acene acene c1cccc1,x
 aphene acene aphene c1ccccc1,x
 mandel|amygdal root root
 C,x,C,x,(,x,0,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Rin
 g,Ring1
 mesit root root
 c,2|o|ortho,Ring,Ring1,c,3|m|meta,(,x,C,alpha1|alpha2|alpha,),x,c,4|p|para,c,5,(
 ,x,C,alpha3|alpha4|alpha',),x,c,6,c,1,(,x,C,alpha5|alpha6|alpha'',),x,Ring,Ring1
 mesitylene|mesitylen root root
 C,alpha1|alpha2|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,C,alpha3|alpha4|
 alpha',),x,c,4|p|para,c,5,(,x,C,alpha5|alpha6|alpha'',),x,c,6,Ring,Ring1
 durene|duren root root
 C,a|alpha|alpha1,c,1,Ring,Ring1,c,2|o|ortho,(,x,C,a'|alpha'|alpha2,),x,c,3|m|met

a,c,4|p|para,(,x,C,a''|alpha''|alpha4,),x,c,5,(,x,C,a'''|alpha'''|alpha5,),x,c,6
 ,Ring,Ring1
 isodurene|isoduren root root
 C,a|alpha|alpha1,c,1,Ring,Ring1,c,2|o|ortho,(,x,C,a'|alpha'|alpha2,),x,c,3|m|met
 a,(,x,C,a''|alpha''|alpha3,),x,c,4|p|para,c,5,(,x,C,a'''|alpha'''|alpha5,),x,c,6
 ,Ring,Ring1
 anisole|anisol root root
 C,a|alpha,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring
 1
 catechol root root
 c,1,Ring,Ring1,(,x,O,o,),x,c,2|ortho,(,x,O,o'),,x,c,3|m|meta,c,4|p|para,c,5,c,6,
 Ring,Ring1
 phenetole|phenetol root root
 C,b|beta,C,a|alpha,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,
 Ring,Ring1
 anethole|anethol root root
 C,x,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(,x,C,x=,x,C,x,C,x,),x
 ,c,5,c,6,Ring,Ring1
 dihydroanethole|dihydroanethol root root
 C,x,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,),x,c,5
 ,c,6,Ring,Ring1
 guaiacol root root
 C,x,O,x,c,2|o|ortho,Ring,Ring1,c,1,(,x,O,x,),x,c,6,c,5,c,4|p|para,c,3|m|meta,Rin
 g,Ring1
 guaiacolate root root
 C,x,O,x,c,2|o|ortho,Ring,Ring1,c,1,(,x,O,1@x,),x,c,6,c,5,c,4|p|para,c,3|m|meta,R
 ing,Ring1
 veratrole|veratrol root root
 C,x,O,x,c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,c,5,c,6
 ,Ring,Ring1
 eugen root root
 c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,C,x=,x
 ,C,x,),x,c,5,c,6,Ring,Ring1
 dihydroeugen root root
 c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,C,x
 ,),x,c,5,c,6,Ring,Ring1
 iso eugen root root
 c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x=,x,C,x
 ,C,x,),x,c,5,c,6,Ring,Ring1
 iso eugenol root root
 O,x,c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x=,x
 ,C,x,C,x,),x,c,5,c,6,Ring,Ring1
 styr|styrene|styrol|cinnamene|cinnamenol|cinnamol root root
 C,b|beta|w|omega=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,
 c,5,c,6,Ring,Ring1
 styral|styral root root
 C,b|beta,(,x,C,a|alpha,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
 c,6,Ring,Ring1
 phosphinine root root
 p,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 anthranil root root
 C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,(,x,N,n,),x,c,3|m|meta,c,4|p|para,c,5,c,6,R
 ing,Ring1
 hippur root trivial
 C,x,C,x,N,x,C,x,(,x=,x,O,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para
 ,c,5,c,6,Ring,Ring1

carbanil loveracid root
C,x,N,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 shikim root root
C,x,C,1,Ring,Ring1,=,x,C,2,C,3,(O),x,C,4,(O),x,C,5,(O),x,C,6,Ring,Ring1
 benzo|benz|dracyl root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 crithmin root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(C),x,c,5,c,6,Ring,Ring1
 dracon root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(OC),x,c,5,c,6,Ring,Ring1
 vanill root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,),x,c,4|p|para,(,x,O,x,),x,c,5,c,6,Ring,Ring1
 isovanill root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(O),x,c,4|p|para,(OC),x,c,5,c,6,Ring,Ring1
 homovanill root root
C,a|alpha,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,),x,c,4|p|para,(,x,O,x,),x,c,5,c,6,Ring,Ring1
 vanillin root root
O,x,Ring,Ring2,,x,O,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 ethylvanillin root root
O,x,Ring,Ring2,,x,O,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OCC),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 isovanillin root root
O,x,Ring,Ring2,,x,O,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,Ring,Ring2,c,4|p|para,(OC),x,c,5,c,6,Ring,Ring1
 acetovanillone root root
O,x,=,x,C,a|alpha,(C),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,),x,c,4|p|para,(,x,O,x,),x,c,5,c,6,Ring,Ring1
 safrole|safrol root root
C,x,=,x,C,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 dihydrosafrole|dihydrosafrol root root
C,x,C,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 isosafrole|isosafrol root root
C,x,C,x,=,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 piperon root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 homopiperon root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 veratr root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|para,(OC),x,c,5,c,6,Ring,Ring1
 homoveratr root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|para,(OC),x,c,5,c,6,Ring,Ring1
 protocatechu root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,),x,c,4|p|para,(,x,O,x,),x,c,5,c,6,Ring,Ring1

homoprotocatechu root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,),x,c,4|p|para,(,x,O,x,),x,c,5,c,6,Ring,Ring1
 citrazin root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,),x,n,4|p|para,c,5,(,x,O,x,),x,c,6,Ring,Ring1
 gall root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,),x,c,4|p|para,(,x,O,x,),x,c,5,(,x,O,x,),x,c,6,Ring,Ring1
 gallacetophenone root root O=C(C)C1=C(O)C(O)=C(O)C=C1,x
 toluene|toluol root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
 cumene|cumen root root
C,x,C,a|alpha,(,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 aniline|anilin|analine|analin root root
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 anilino|analino root root
N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 gentis root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,(,x,O,o',),x,c,6,Ring,Ring1
 homogentis root root
C,x,C,x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,(,x,O,o'),,x,c,6,Ring,Ring1
 salicyl|salic root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 salicylal root root
C,8@x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 anilot root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,([N+] (=O) [O-]),x,c,6,Ring,Ring1
 alpharesorcyl|aresorcyl root root
C,x,c,1,Ring,Ring1,c,2,c,3|m|meta,(,x,O,x,),x,c,4|p|para,c,5,(,x,O,x,),x,c,6,Ring,Ring1
 betaresorcyl|bresorcyl root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,x,),x,c,3|m|meta,c,4|p|para,(,x,O,x,),x,c,5,c,6,Ring,Ring1
 gammaresocryl|gresocryl root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,x,),x,c,3|m|meta,c,4|p|para,c,5,c,6,(,x,O,x,),x,Ring,Ring1
 phenac root root
C,a|alpha,C,x,(,x,=,x,O,x,),x,c,x,Ring,Ring1,=,x,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 trop root root
C,x,C,x,(,x,C,x,O,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 nortrop root root
C,x,(,x,C,x,O,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 hydratrop root root
C,x,C,x,(,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 homatrop root root CN1C2CCCC1CC(OC(C(O)C3=CC=CC=C3)=O)C2,x
 atrop root root OCC(C(OC3CC2CCC(C3)N2C)=O)c1cccc1,x

tropan|tropane root root C,3,(,x,C,2,C,1,Ring,Ring1,Ring,Ring2,),x,C,4,C,5|alpha-,
 r,(,x,C,6|alpha-b,C,7|alpha-t,Ring,Ring2,),x,N,8,Ring,Ring1,C,x
 tropin|tropine root root C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,(O),x,C,4,C,5|alpha-,
 r,(,x,C,6|alpha-b,C,7|alpha-t,Ring,Ring2,),x,N,8,Ring,Ring1,C,x
 1alphah5alphahtropan root root
 C,3,(,x,C,2,[C@],1,([H]),x,Ring,Ring1,Ring,Ring2,),x,C,4,[C@],5|alpha-,
 r,([H]),x,(,x,C,6|alpha-b,C,7|alpha-t,Ring,Ring2,),x,N,8,Ring,Ring1,C,x
 tropinone root root CN1C(C2)CCC1CC2=O,x
 atrolact root root
 C,x,C(C)(O),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 cinnamo|cinnam root root
 C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
 c,6,Ring,Ring1
 cinnamal root root
 C,8@x,C,a|alpha,=,x,C,b|beta:c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,
 5,c,6,Ring,Ring1
 hydrocinnam root root
 C,x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,
 6,Ring,Ring1
 hydrocinnamal root root
 C,8@x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,
 6,Ring,Ring1
 grevill root root
 C,x,/,x,C,a|alpha,=,x,C,b|beta,/,x,c,1,Ring,Ring1,c,2|o|ortho,(O),x,c,3|m|meta,c,
 4|p|para,c,5,(O),x,c,6,Ring,Ring1
 caffe root root
 C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(O),x,c,4|p|par
 a,(O),x,c,5,c,6,Ring,Ring1
 ferul root root
 C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
 ra,(O),x,c,5,c,6,Ring,Ring1
 sinap root root
 C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
 ra,(O),x,c,5,(OC),x,c,6,Ring,Ring1
 conifer|conifero root root
 C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
 ra,(O),x,c,5,c,6,Ring,Ring1
 phloret root root
 C,x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(O),x,c,
 5,c,6,Ring,Ring1
 nicotino|nicotine|nicotin loveracid root
 C,x,c,3,Ring,Ring1,c,4,c,5,c,6,n,1,c,2,Ring,Ring1
 nicotin root root C,x,c,3,Ring,Ring1,c,4,c,5,c,6,n,1,c,2,Ring,Ring1
 isonicotino|isonicotin root root
 C,x,c,4,Ring,Ring1,c,5,c,6,n,1,c,2|alpha|beta,c,3|beta|alpha,Ring,Ring1
 melamine|melamin root root
 n,1,Ring,Ring1,c,2,(N),x,n,3,c,4,(N),x,n,5,c,6,(N),x,Ring,Ring1
 pyrylium root root
 [o+],1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 naphtho|naphth|naphthalene|naphthalen root root
 c,1|alpha|Ring,Ring1,c,2|beta|beta,c,3,c,4,c,4a|4alpha|Ring,Ring2,c,5,c,6,c,7,c,8
 ,c,8a|8alpha|Ring,Ring1,Ring,Ring2
 naphtho|naphth opfuser unknown
 c,1|alpha|Ring,Ring1,c,2|beta|beta,c,3,c,4,c,4a|4alpha|Ring,Ring2,c,5,c,6,c,7,c,8
 ,c,8a|8alpha|Ring,Ring1,Ring,Ring2

naphtho-quinone|naphtho-quinon|naphthalene-quinone|naphthalene-quinon root root
 c,1|a|alpha, (=O), x, Ring, Ring1, c,2|b|beta, =, x, c, 3, c, 4, (=O), x, c, 4a|4alpha, Ring, Ring1, c, 5, c, 6, c, 7, c, 8, c, 8a|8alpha, Ring, Ring1, Ring, Ring2
 cadalene|cadalen root root
 c,1|a|alpha, (C), x, Ring, Ring1, c,2|b|beta, c, 3, c, 4, (C(C)C), x, c, 4a|4alpha, Ring, Ring2, c, 5, c, 6, (C), x, c, 7, c, 8, c, 8a|8alpha, Ring, Ring1, Ring, Ring2
 benzodioxene|benzodioxen root root
 o,1, Ring, Ring1, c,2, c,3, o,4, c, 4a|4alpha, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a|8alpha, Ring, Ring1, Ring, Ring2
 azulene|azulen root root
 c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
 azuleno|azulen opfuser unknown
 c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
 anthracene|anthracen|anthro|anthr root root
 c,1|a|alpha, Ring, Ring1, c,2|b|beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 10, c, 5a|10a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 9, c, 9a, Ring, Ring2, Ring, Ring1
 anthrone|anthron root root
 c,1|a|alpha, Ring, Ring1, c,2|b|beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 10, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 9, (=, x, O, x,), x, c, 9a, Ring, Ring2, Ring, Ring1
 anthra-quinone|anthra-quinon|anthracene-quinone|anthracene-quinon root root
 c,1|a|alpha, Ring, Ring1, c,2|b|beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 10, (=O), x, c, 5a|10a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 9, (=, x, O, x,), x, c, 9a, Ring, Ring2, Ring, Ring1
 anthra|anthraceno opfuser unknown
 c,1|a|alpha, Ring, Ring1, c,2|b|beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 10, c, 5a|10a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 9, c, 9a, Ring, Ring2, Ring, Ring1
 acrid root root
 c,1|a|alpha, Ring, Ring1, c,2|b|beta, c, 3, c, 4, c, 4a, Ring, Ring2, n, 10, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 9, c, 9a, Ring, Ring2, Ring, Ring1
 aminacrine|aminacrin|aminacridin|aminacridine|monacrin|monacrine root root
 c,1|a|alpha, Ring, Ring1, c,2|b|beta, c, 3, c, 4, c, 4a, Ring, Ring2, n, 10, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 9, (N), n, c, 9a, Ring, Ring2, Ring, Ring1
 acenaphthene|acenaphthen root root
 C,1, Ring, Ring1, C,2, c, 2a, Ring, Ring2, c, 3, c, 4, c, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, c, 8b, Ring, Ring2, Ring, Ring3
 acenaphtho|acenaphth opfuser unknown
 C,1, Ring, Ring1, C,2, c, 2a, Ring, Ring2, c, 3, c, 4, c, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, c, 8b, Ring, Ring2, Ring, Ring3
 acenaphthylene|acenaphthylen root root
 c,1, Ring, Ring1, c,2, c, 2a, Ring, Ring2, c, 3, c, 4, c, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, c, 8b, Ring, Ring2, Ring, Ring3
 cholanthrene|cholanthren root root
 C,1, Ring, Ring1, C,2, c, 2a, Ring, Ring2, c, 3, c, 4, c, 5, c, 5a, Ring, Ring3, c, 6, c, 6a, Ring, Ring4, c, 6b, Ring, Ring5, c, 7, c, 8, c, 9, c, 10, c, 10a, Ring, Ring5, c, 11, c, 12, c, 12a, Ring, Ring4, c, 12b, Ring, Ring1, c, 12c, Ring, Ring3, Ring, Ring2
 phenalene|phenalen root root
 c,1, Ring, Ring1, c,2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 6a, Ring, Ring3, c, 7, c, 8, c, 9, c, 9a, Ring, Ring1, c, 9b, Ring, Ring2, Ring, Ring3
 julolid root root
 C,1, Ring, Ring1, C,2, c, C, N, 4, Ring, Ring2, C, 5, C, 6, C, 7, c, 7a, Ring, Ring3, c, 8, c, 9, c, 10, c, 10a, Ring, Ring1, c, 10b, Ring, Ring2, Ring, Ring3
 perimid root root
 n,1, Ring, Ring1, c,2, n, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 6a, Ring, Ring3, c, 7, c, 8, c, 9, c, 9a, Ring, Ring1, c, 9b, Ring, Ring2, Ring, Ring3

phenanthren|phenanthrene root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,4b,Ring, Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3,c,9,c,10,c,10a,Ring, Ring1,Ring, Ring2
phenantr|phenanthro|phenanthra opfuser unknown
c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,4b,Ring, Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3,c,9,c,10,c,10a,Ring, Ring1,Ring, Ring2
cyclopentadefphenanthren|cyclopentadefphenanthrene root root
c,1,Ring, Ring1,c,2,c,3,c,3a,Ring, Ring2,c,4,c,4a,Ring, Ring3,c,5,c,6,c,7,c,7a,Ring
,Ring4,c,8,c,9,c,8a,Ring, Ring1,c,8b,Ring, Ring2,c,8c,Ring, Ring3,Ring, Ring4
bathophenanthroline root root
n,1,Ring, Ring1,c,2,c,3,c,4,(c4cccc4),x,c,4a,Ring, Ring2,c,5,c,6,c,6a,Ring, Ring3,
c,7,(c5ccccc5),x,c,8,c,9,n,10,c,10a,Ring, Ring3,c,10b,Ring, Ring1,Ring, Ring2
phenanthrone|phenanthron root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,4b,Ring, Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3,C,9,(=O),x,C,10,c,10a,Ring, Ring1,Ring, Ring2
phenanthrene-quinone|phenanthrene-quinon root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,4b,Ring, Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3,c,9,(=O),x,c,10,(=O),x,c,10a,Ring, Ring1,Ring, Ring2
cyclopentaaphenanthrene|cyclopentaaphenanthren root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,5,Ring, Ring2,c,6,c,7,c,8,Ring, Ring3,c,14,Ring, Ring4
,c,15,c,16,c,17,c,13,Ring, Ring4,c,12,c,11,c,9,Ring, Ring3,c,10,Ring, Ring2,Ring, Ri
ng1
fluoranthene|fluoranth|fluoranthen root root
c,1,Ring, Ring1,c,2,c,3,c,3a,Ring, Ring2,c,4,c,5,c,6,c,6a,Ring, Ring3,c,6b,Ring, Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring, Ring4,c,10b,Ring, Ring1,c,10c,Ring, Ring2,Ring, Ring
3
acephenanthrene|acephenanthren root root
c,1,Ring, Ring1,c,2,c,3,c,3a,Ring, ring2,C,4,C,5,c,5a,Ring, Ring3,c,6,c,6a,Ring, rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring, Ring4,c,10b,Ring, Ring1,c,10c,Ring, Ring2,Ring, Ring
3
acephenanthrylene|acephenanthrylen root root
c,1,Ring, Ring1,c,2,c,3,c,3a,Ring, ring2,c,4,c,5,c,5a,Ring, Ring3,c,6,c,6a,Ring, rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring, Ring4,c,10b,Ring, Ring1,c,10c,Ring, Ring2,Ring, Ring
3
aceanthrene|aceanthren root root
C,1,Ring, Ring1,C,2,c,2a,Ring, Ring2,c,3,c,4,c,5,c,5a,Ring, Ring3,c,6,c,6a,Ring, Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring, Ring4,c,10b,Ring, Ring1,c,10c,Ring, Ring2,Ring, Ring
3
aceanthrylene|aceanthrylen root root
c,1,Ring, Ring1,c,2,c,2a,Ring, Ring2,c,3,c,4,c,5,c,5a,Ring, Ring3,c,6,c,6a,Ring, Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring, Ring4,c,10b,Ring, Ring1,c,10c,Ring, Ring2,Ring, Ring
3
violanthrene|violanthren root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,C,5,c,5a,Ring, Ring3,c,6,c,7,c,7a,Ring
,Ring4,c,7b,Ring, Ring5,c,8,c,9,c,9a,(,x,c,18f,Ring, Ring6,c,18e,Ring, Ring7,Ring, R
ing5,),x,C,10,c,10a,Ring, Ring8,c,11,c,12,c,13,c,14,c,14a,Ring, Ring8,c,14b,Ring, R
ing6,c,15,c,16,c,16a,Ring, Ring7,c,16b,Ring, Ring9,c,17,c,18,c,18a,(,x,c,18b,Ring,
Ring1,Ring, Ring2,),x,c,18c,Ring, Ring3,c,18d,Ring, Ring4,Ring, Ring9
isoviolanthrene|isoviolanthren root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,4b,Ring, Ring3,c,5,c,6,c,6a,(,x,c,18
c,Ring, Ring4,c,18b,Ring, Ring5,Ring, Ring3,),x,c,6b,Ring, Ring6,c,7,c,8,c,8a,(,x,c,
18e,Ring, Ring7,c,18d,Ring, Ring8,Ring, Ring6,),x,C,9,c,9a,Ring, Ring9,c,10,c,11,c,1
2,c,13,c,13a,Ring, Ring9,c,13b,Ring, Ring7,c,14,c,15,c,15a,Ring, Ring8,c,15b,Ring, R
ing4,c,16,c,17,c,17a,Ring, Ring5,C,18,c,18a,Ring, Ring1,Ring, Ring2
triphenylene|triphenylen root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,4b,Ring, Ring3,c,5,c,6,c,7,c,8,c,8a,

Ring,Ring3,c,8b,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,c,12b,Ring,Ring2,
 Ring,Ring1
 trindene|trinden root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,3b,Ring,Ring3,c,4,c,5,c,6,c,6a,Ring,Rin
 g3,c,6b,Ring,Ring4,c,7,c,8,c,9,c,9a,Ring,Ring4,c,9b,Ring,Ring2,Ring,Ring1
 pyrene|pyren root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
 Ring,Ring4,c,9,c,10,c,10a,Ring,Ring1,c,10b,Ring,Ring2,c,10c,Ring,Ring3,Ring,Ring
 4
 chrysene|chrysen root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,6a,Ring,Rin
 g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring3,c,11,c,12,c,12a,Ring,Ring2
 ,Ring,Ring1
 naphthacene|naphthacen root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
 g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,11,c,11a,Ring,Ring3,c,12,c,12a,Ring,Ring2
 ,Ring,Ring1
 naphthaceno|naphthacen opfuser unknown
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
 g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,11,c,11a,Ring,Ring3,c,12,c,12a,Ring,Ring2
 ,Ring,Ring1
 pleiadene|pleiaden root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,7a,Ring
 ,Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,12,c,12a,Ring,Ring1,c,12b,Ring,Ring3
 ,Ring,Ring2
 picene|picen root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Rin
 g4,c,7,c,8,c,8a,Ring,Ring5,c,9,c,10,c,11,c,12,c,12a,Ring,Ring5,c,12b,Ring,Ring4,
 c,13,c,14,c,14a,Ring,Ring3,c,14b,Ring,Ring2,Ring,Ring1
 perylene|perylene root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Rin
 g4,c,7,c,8,c,9,c,9a,Ring,Ring5,c,10,c,11,c,12,c,12a,(,x,c,12d,Ring,Ring5,Ring,Ri
 ng4,),x,c,12b,Ring,Ring1,c,12c,Ring,Ring2,Ring,Ring3
 perylo opfuser unknown
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Rin
 g4,c,7,c,8,c,9,c,9a,Ring,Ring5,c,10,c,11,c,12,c,12a,(,x,c,12d,Ring,Ring5,Ring,Ri
 ng4,),x,c,12b,Ring,Ring1,c,12c,Ring,Ring2,Ring,Ring3
 tetraphenylene|tetraphenyl root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
 Ring,Ring3,c,8b,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,c,12b,Ring,Ring5,
 c,13,c,14,c,15,c,16,c,16a,Ring,Ring5,c,16b,Ring,Ring2,Ring,Ring1
 rubicene|rubicen root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,3b,Ring,Ring3,c,4,c,5,c,6,c,7,c,7a,Ring
 ,Ring3,c,7b,Ring,Ring4,c,7c,Ring,Ring5,c,8,c,9,c,10,c,10a,Ring,Ring6,c,10b,Ring,
 Ring7,c,11,c,12,c,13,c,14,c,14a,Ring,Ring7,c,14b,(,x,c,14e,Ring,Ring6,Ring,Ring5
 ,),x,c,14c,Ring,Ring1,c,14d,Ring,Ring2,Ring,Ring4
 coronene|coronen root root
 c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,4a,Ring,Ring3,c,5,c,6,c,6a,Ring,Rin
 g4,c,7,c,8,c,8a,Ring,Ring5,c,9,c,10,c,10a,Ring,Ring6,c,11,c,12,c,12a,Ring,Ring1,
 c,12b,Ring,Ring7,c,12c,Ring,Ring2,c,12d,Ring,Ring3,c,12e,Ring,Ring4,c,12f,Ring,R
 ing5,c,12g,Ring,Ring6,Ring,Ring7
 trinaphthylene|trinaphthylen root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,5b,Ring,Ring4,c
 ,6,c,6a,Ring,Ring5,c,7,c,8,c,9,c,10,c,10a,Ring,Ring5,c,11,c,11a,Ring,Ring4,c,11b
 ,Ring,Ring6,c,12,c,12a,Ring,Ring7,c,13,c,14,c,15,c,16,c,16a,Ring,Ring7,c,17,c,17
 a,Ring,Ring6,c,17b,Ring,Ring3,c,18,c,18a,Ring,Ring2,Ring,Ring1

pyranthrene|pyranthren root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,4b,Ring, Ring3,c,5,c,5a,Ring, Ring4,c,6,c,7,c,7a,Ring, Ring5,c,8,c,8a,Ring, Ring6,c,9,c,10,c,11,c,12,c,12a,Ring, Ring7,c,12b,Ring, Ring8,c,13,c,13a,Ring, Ring9,c,14,c,15,c,15a,(,x,c,16,c,16a,Ring, Ring2,Ring, Ring1,),,x,c,15b,Ring, Ring3,c,15c,Ring, Ring8,c,15d,Ring, Ring4,c,15e,Ring, Ringg7,Ring, Ring5
 ovalene|ovalen root root
 c,1,Ring, Ring1,c,2,c,2a,Ring, Ring2,c,3,c,4,c,4a,Ring, Ring3,c,5,c,6,c,6a,Ring, Ringg4,c,7,c,7a,Ring, Ring5,c,8,c,9,c,9a,Ring, Ring6,c,10,c,11,c,11a,Ring, Ring7,c,12,c,13,c,13a,Ring, Ring8,c,14,c,14a,Ring, Ring1,c,14b,Ring, Ring9,c,14c,Ring, Ring2,c,14d,Ring, Ring3,c,14e,Ring, Ring4,c,14f,Ring, Ring0,c,14g,Ring, Ring5,c,14h,Ring, Ring6,c,14i,Ring, Ring7,c,14j,Ring, Ring8,c,14k,Ring, Ring0,Ring, Ring9
 biphenylene|biphenylen root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,4b,Ring, Ring3,c,5,c,6,c,7,c,8,c,8a,Ring, Ring3,c,8b,Ring, Ring2,Ring, Ring1
 thianthrene|thianthren root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,s,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c,9a,Ring, Ring3,s,10,c,10a,Ring, Ring2,Ring, Ring1
 pyr root root
 c,2|a|alpha,Ring, Ring1,c,3 b|beta,c,4|g|gamma,c,5,c,6,o,1,Ring, Ring1
 pyrano opfuser unknown c,2,Ring, Ring1,c,3,c,4,c,5,c,6,o,1,Ring, Ring1
 mdioxine|mdioxin root root c,2,Ring, Ring1,o,3,c,4,c,5,c,6,o,1,Ring, Ring1
 pdioxine|pdioxin root root c,2,Ring, Ring1,c,3,o,4,c,5,c,6,o,1,Ring, Ring1
 oxalene|oxalen root root
 c,1,Ring, Ring1,c,2,c,3,c,3a,Ring, Ring2,c,4,c,5,c,6,o,7,c,7a,Ring, Ring2,Ring, Ring1
 azalene|azalen root root
 c,1,Ring, Ring1,c,2,c,3,c,3a,Ring, Ring2,c,4,c,5,c,6,n,7,c,7a,Ring, Ring2,Ring, Ring1
 isobenzofuran root root
 c,1,Ring, Ring1,o,2,c,3,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring2,Ring, Ring1
 benzofurazan root root
 n,1,Ring, Ring1,o,2,n,3,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring2,Ring, Ring1
 benzofuroxan root root [n+],1,(,x,[O-],,x,,Ring, Ring1,o,2,n,3,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring2,Ring, Ring1
 piazthiole root root
 n,1,Ring, Ring1,s,2,n,3,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring2,Ring, Ring1
 catecholborane root root
 o,x,Ring, Ring1,B,b,o,x,c,2,Ring, Ring2,c,3,c,4,c,5,c,6,c,1,Ring, Ring2,Ring, Ring1
 chromene|chromen root root
 c,2,Ring, Ring1,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring2,o,1,Ring, Ring1
 chromane|chroman root root
 C,2,Ring, Ring1,C,3,C,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring2,O,1,Ring, Ring1
 chromone|chromon root root
 c,2,Ring, Ring1,c,3,c,4,(=O),x,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring2,o,1,Ring, Ring1
 esculetin root root
 c,2,Ring, Ring1,(=O),x,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,(O),x,c,7,(O),x,c,8,c,8a,Ring, Ring2,o,1,Ring, Ring1

umbelliferone root root
 c,2,Ring,Ring1,(=O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ri
 ng2,o,1,Ring,Ring1
 umbelliferyl root root
 c,2,Ring,Ring1,(=O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,4@7,c,8,c,8a,Ring,Ring2,
 o,1,Ring,Ring1
 isochromane|isochroman root root
 C,1,Ring,Ring1,O,2,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
 Ring2
 flav root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,C,4|a-
 l,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,O,1,Ring,Ring1,),x,c,1',Ring,R
 ing3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 flavone|flavon root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x,c,1'
 ,Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 acacetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(OC),x,c,5',c,6',Ring,Ring3
 alpinetin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(OC),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 apigenin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
 baicalein root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(O),x,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,R
 ing,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 catechin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,(O),x,C,4|a-
 l,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x
 ,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
 chrysin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3
 cirsiliol root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(OC),x,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1
 ,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
 diosmetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
 epicatechin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,(O),x,C,4|a-
 l,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x
 ,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
 eupatorin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(OC),x,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1
 ,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
 galangin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 genkwanin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
 hesperitin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
 kaempferide|kaempferol root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3

luteolin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
 morin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
 myricetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',(O),x,c,6',Ring,Ring3
 naringenin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
 pinocembrin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 pinostrobin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 quercetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
 robinetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),
 x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',(O),x,c,6',Ring,Ring3
 sinensetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(OC),x,c,6,(OC),x,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,
 1,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(OC),x,c,5',c,6',Ring,Rin
 g3
 syringetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3
 tectochrysin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 isoflavone|isoflavan root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x,c,1'
 ,Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 daidzein root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),
 x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
 formononetin root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),
 x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
 genistein root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-
 1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
 flavyllum root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,),x,c,1',Rin
 g,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 malvidin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 1,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,
),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3
 cyanidin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
 1,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,
),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3

flavanone|flavanon root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,C,4|a-
 l,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,O,1,Ring,Ring1,),x,c,1'
 ,Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 anaphthoflavone|anaphthoflavon|alphanaphthoflavone|alphanaphthoflavon root root
 O=C2C=C(C4=CC=CC=C4)OC1=C3C(C=CC=C3)=CC=C12,x
 bnaphthoflavone|bnaphthoflavon|betanaphthoflavone|betanaphthoflavon root root
 O=C2C=C(C3=CC=CC=C3)OC1=CC=C4C(C=CC=C4)=C12,x
 xanthene|xanthen|xanthhydr|xanth root root
 c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,10,c,10a,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
 xanthone|xanthon root root
 c,9,Ring,Ring1,(,x,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,10,c,10a,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
 xanthylum root root
 c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,[o+],10,c,10a,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
 xanthuren root root
 C,x,c,2,Ring,Ring1,c,3,c,4,(O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,(O),x,c,8a,Ring,Ring2,n,1,Ring,Ring1
 thioxanthene|thioxanthen root root
 c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,10,c,10a,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
 selenoxanthene|selenoxanthen root root
 c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,[se],10,c,10a,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
 acridars root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,c,10,c,10a,Ring,Ring2,Ring,Ring1
 arsanthrene|arsanthren root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
 phosphanthrene|phosphanthren root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,p,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,p,10,c,10a,Ring,Ring2,Ring,Ring1
 selenanthrene|selenanthren root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[se],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,[se],10,c,10a,Ring,Ring2,Ring,Ring1
 phenomericurin root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[Hg],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,[Hg],10,c,10a,Ring,Ring2,Ring,Ring1
 phenoxyathiin root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,s,10,c,10a,Ring,Ring2,Ring,Ring1
 phenoxyastannin root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,[Sn],10,c,10a,Ring,Ring2,Ring,Ring1
 phenoxyasilin root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,[Si],10,c,10a,Ring,Ring2,Ring,Ring1
 phenoxygermanin root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,[Ge],10,c,10a,Ring,Ring2,Ring,Ring1
 phenoxytannin root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,S,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c,9a,Ring,Ring3,[Sn],10,c,10a,Ring,Ring2,Ring,Ring1

phenothiasilin root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,S,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[Si],10,c,10a,Ring, Ring2,Ring, Ring1
 phenothiagermanin root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,S,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[Ge],10,c,10a,Ring, Ring2,Ring, Ring1
 phenaz root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,n,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,n,10,c,10a,Ring, Ring2,Ring, Ring1
 phenazasiline|phenazasilin root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,N,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[Si],10,c,10a,Ring, Ring2,Ring, Ring1
 phenarsaz|phenoarsaz root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,n,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[as],10,c,10a,Ring, Ring2,Ring, Ring1
 phenothiaz|thiodiphenylamine root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,s,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,n,10,c,10a,Ring, Ring2,Ring, Ring1
 phenomercaz root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,N,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[Hg],10,c,10a,Ring, Ring2,Ring, Ring1
 phenophosphaz root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,n,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,p,10,c,10a,Ring, Ring2,Ring, Ring1
 phenotelluraz root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,[Te],5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,
 9,c,9a,Ring, Ring3,N,10,c,10a,Ring, Ring2,Ring, Ring1
 phenoselenaz root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,[Se],5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,
 9,c,9a,Ring, Ring3,N,10,c,10a,Ring, Ring2,Ring, Ring1
 phenothiars root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,s,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[as],10,c,10a,Ring, Ring2,Ring, Ring1
 phenoxantimon root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,O,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[Sb],10,c,10a,Ring, Ring2,Ring, Ring1
 phenoxars root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,o,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[as],10,c,10a,Ring, Ring2,Ring, Ring1
 phenoxaphos root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,O,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,P,10,c,10a,Ring, Ring2,Ring, Ring1
 phenoxatellur root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,O,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[Te],10,c,10a,Ring, Ring2,Ring, Ring1
 phenoxaselen root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,O,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,[Se],10,c,10a,Ring, Ring2,Ring, Ring1
 dibenzodioxin root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,o,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,o,10,c,10a,Ring, Ring2,Ring, Ring1
 phenoxaz|phenazox root root
 c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,o,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring, Ring3,n,10,c,10a,Ring, Ring2,Ring, Ring1
 indene|inden root root
 c,1,Ring, Ring1,c,2,c,3,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring1,Ring, Ring2

indeno opfuser unknown
 c,1,Ring, Ring1, c,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, Ring
 2
 indole|indol root root
 n,1,Ring, Ring1, c,2|a|alpha, c,3|b|beta, c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring1, Ring, Ring2
 thianaphthene|thianaphthen|thionaphthene|thionaphthen root root
 s,1,Ring, Ring1, c,2|a|alpha, c,3|b|beta, c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring1, Ring, Ring2
 thianaphtheno|thianaphthen opfuser unknown
 s,1,Ring, Ring1, c,2|a|alpha, c,3|b|beta, c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring1, Ring, Ring2
 isothianaphthene|isothianaphthen root root
 c,1,Ring, Ring1, s,2|a|alpha, c,3|b|beta, c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring1, Ring, Ring2
 isothianaphtheno|isothianaphthen opfuser unknown
 c,1,Ring, Ring1, s,2|a|alpha, c,3|b|beta, c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring1, Ring, Ring2
 skatole|skatol root root
 n,1,Ring, Ring1, c,2,c,3,(C),x,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Rin
 g, Ring2
 gramine root root
 n,1,Ring, Ring1, c,2,c,3,(CN(C)C),x,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring
 1, Ring, Ring2
 indolo opfuser unknown
 n,1,Ring, Ring1, c,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, Ring
 2
 isoindole|isoindol root root
 c,1,Ring, Ring1, n,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, Ring
 2
 isoindolo opfuser unknown
 c,1,Ring, Ring1, n,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, Ring
 2
 arsindole|arsindol root root
 [as],1,Ring, Ring1, c,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, R
 ing2
 arsindolo opfuser unknown
 [as],1,Ring, Ring1, c,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, R
 ing2
 isoarsindole|isoarsindol root root
 c,1,Ring, Ring1, [as],2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, R
 ing2
 isoarsindolo|isoarsindol opfuser unknown
 c,1,Ring, Ring1, [as],2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, R
 ing2
 phosphindole|arsindol root root
 p,1,Ring, Ring1, c,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, Ring
 2
 phosphindolo|arsindol opfuser unknown
 p,1,Ring, Ring1, c,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, Ring
 2
 isophosphindole|isoarsindol root root
 c,1,Ring, Ring1, p,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, Ring
 2
 isophosphindolo|isoarsindol opfuser unknown
 c,1,Ring, Ring1, p,2,c,3,c,3a,Ring, Ring2, c,4,c,5,c,6,c,7,c,7a,Ring, Ring1, Ring, Ring
 2

indazole|indazol root root
 n,1,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 indazolo|indazol opfuser unknown
 n,1,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 indolizine|indolizin|pyrrocol root root
 c,1,Ring,Ring1,c,2,c,3,n,4,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
 indolizino opfuser unknown
 c,1,Ring,Ring1,c,2,c,3,n,4,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
 oxindole|oxindol root root
 N,1,Ring,Ring1,C,2,(=,x,O,x,),x,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 indoline|indolin root root
 N,1,Ring,Ring1,C,2,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 isat root root
 N,1,Ring,Ring1,C,2|alpha,(=O),x,C,3|beta,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 isoindoline|isoindolin root root
 C,1,Ring,Ring1,N,2,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 indane|indan|hydrindene|hydrind root root
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 hydrindantin root root O=C(c2c1cccc2)C(C1=O)(O)C(C3=O)(O)C(c4c3cccc4)=O,x
 alloxantin root root OC1(C2(C(NC(NC2=O)=O)=O)O)C(NC(NC1=O)=O)=O,x
 ninhydrin root root
 C,1,(=O),x,Ring,Ring1,C,2,(=O),x,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring2
 tetral root root
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
 decal root root
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,C,4,C,10,Ring,Ring2,c,5,C,6,C,7,C,8,C,9,Ring,Ring1,Ring,Ring2
 hexalin root root C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1
 quinol|chinol|quinolin|chinolin|leucol root root
 n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
 quinolin|chinolin opfuser unknown
 n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
 carbostyryl|carbostyryl root root
 n,1,Ring,Ring1,c,2|b|beta,(O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
 isocarbostyryl|isocarbostyryl root root
 c,1,(O),x,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
 lepid root root
 n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,(C),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
 cinchonin loveracid root
 c,4,Ring,Ring1,c,3,c,2,n,1,c,8a,Ring,Ring2,c,8,c,7,c,6,c,5,c,4a,Ring,Ring1,Ring,Ring2

quino|chino opfuser unknown
 n,1,Ring, Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring
 1,Ring, Ring2
 quinald|chinald root root
 C,a|alpha,Ring, Ring, Ring3,..x,n,1,Ring, Ring1,c,2|b|beta,Ring, Ring3,c,3,c,4,c,4a,Ring,
 Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring1, Ring, Ring2
 xanthur root root
 C,a|alpha,Ring, Ring3,..x,n,1,Ring, Ring1,c,2|b|beta,Ring, Ring3,c,3,c,4,(O),x,c,4a
 ,Ring, Ring2,c,5,c,6,c,7,c,8,(O),x,c,8a,Ring, Ring1, Ring, Ring2
 quinoliz|chinoliz root root
 c,1,Ring, Ring1,c,2,c,3,c,4,n,5,Ring, Ring2,c,6,c,7,c,8,c,9,c,8a,Ring, Ring2,Ring, R
 ing1
 quinazol|chinazol root root
 n,1,Ring, Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring
 1,Ring, Ring2
 quinazol|chinazol|quinazolino opfuser unknown
 n,1,Ring, Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring
 1,Ring, Ring2
 isoquinol|isochinol root root
 c,1|a|alpha,Ring, Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,R
 ing, Ring1, Ring, Ring2
 isoquino|isochino opfuser unknown
 c,1|a|alpha,Ring, Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,R
 ing, Ring1, Ring, Ring2
 cinnol root root
 n,1,Ring, Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring
 1,Ring, Ring2
 quinoxal|chinoxal|phenpiaz root root
 n,1,Ring, Ring1,c,2|b|beta,c,3,n,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring
 1,Ring, Ring2
 arsinol root root
 [as],1,Ring, Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, R
 ing1, Ring, Ring2
 isoarsinol root root
 c,1|a|alpha,Ring, Ring1,[as],2|b|beta,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8
 a,Ring, Ring1, Ring, Ring2
 phosphinol root root
 p,1,Ring, Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring
 1,Ring, Ring2
 isophosphiol root root
 c,1|a|alpha,Ring, Ring1,p,2|b|beta,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,R
 ing, Ring1, Ring, Ring2
 pterid root root
 n,1,Ring, Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring, Ring2,n,5,c,6,c,7,n,8,c,8a,Ring, Ring
 1,Ring, Ring2
 phthalazine|phthalazin root root
 c,1|a|alpha,Ring, Ring1,n,2|b|beta,n,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,R
 ing, Ring1, Ring, Ring2
 phthalhydrazide root root
 C,x,Ring, Ring1,(=O),x,N,x,N,x,C,x,(=O),x,c,2,Ring, Ring2,c,3,c,4,c,5,c,6,c,1,Ring
 ,Ring1, Ring, Ring2
 fluorene|fluoren root root
 c,9,Ring, Ring1,c,9a,Ring, Ring2,c,1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,5a,Ring, Ring3,c
 ,5,c,6,c,7,c,8,c,8a,Ring, Ring3,Ring, Ring1
 diphenyleneiodonium root root
 [I+],9,Ring, Ring1,c,9a,Ring, Ring2,c,1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,5a,Ring, Ring
 3,c,5,c,6,c,7,c,8,c,8a,Ring, Ring3,Ring, Ring1

betacarboline root root
 c,1,Ring,Ring1,n,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
 Ring,Ring3,n,9|prefhydro,c,9a,Ring,Ring2,Ring,Ring1
 carbazole|carbazol root root
 n,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring3,c
 ,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
 carbazolo|carbazol opfuser unknown
 n,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring3,c
 ,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
 norharman root root
 n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,n,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ri
 ng,Ring3,c,5,c,6,c,7,c,8a,Ring,Ring3,Ring,Ring1
 harmane|harman root root
 n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
 ,5a,Ring,Ring3,c,5,c,6,c,7,c,8a,Ring,Ring3,Ring,Ring1
 harmine|banisterine root root
 n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
 ,5a,Ring,Ring3,c,5,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
 harmol root root
 n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
 ,5a,Ring,Ring3,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
 harmalol root root
 N,9,Ring,Ring1,C,9a,Ring,Ring2,C,1,(C),x,=,x,N,2,C,3,C,4,C,4a,(,x,=,x,Ring,Ring2
),x,c,4b,Ring,Ring3,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
 harmaline root root
 n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
 ,5a,Ring,Ring3,c,5,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
 harmalane|harmalan root root
 n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
 ,5a,Ring,Ring3,c,5,c,6,(OC),x,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
 phenanthrid root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
 ,10,c,10a,Ring,Ring3,c,10b,Ring,Ring2,Ring,Ring1
 arsanthrid root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,
 9,c,10,c,10a,Ring,Ring3,c,10b,Ring,Ring2,Ring,Ring1
 benzidine|benzidin root root
 N,n,c,4,Ring,Ring1,c,3,c,2,c,1,(,x,c,6,c,5,Ring,Ring1,),x,c,1',Ring,Ring2,c,2',c
 ,3',c,4',(,x,N,n',),x,c,5',c,6',Ring,Ring2
 benzidinium root root
 [N+],n,c,4,Ring,Ring1,c,3,c,2,c,1,(,x,c,6,c,5,Ring,Ring1,),x,c,1',Ring,Ring2,c,2
 ',c,3',c,4',(,x,[N+],n',),x,c,5',c,6',Ring,Ring2
 benzidino root root
 N,4@n,c,4,Ring,Ring1,c,3,c,2,c,1,(,x,c,6,c,5,Ring,Ring1,),x,c,1',Ring,Ring2,c,2'
 ,c,3',c,4',(,x,N,n',),x,c,5',c,6',Ring,Ring2
 pyrid root root
 c,2|o|ortho|a|alpha,Ring,Ring1,c,3|m|meta|b|beta,c,4|p|para|g|gamma,c,5,c,6,n,1|
 n,Ring,Ring1
 pyrido|pyrid opfuser unknown
 c,2|o|ortho|a|alpha,Ring,Ring1,c,3|m|meta|b|beta,c,4|p|para|g|gamma,c,5,c,6,n,1|
 n,Ring,Ring1
 pyridox root root
 C,4,c,x,Ring,Ring1,c,x,(,x,C,5,O,x,),x,c,6,n,1,c,2,(C),x,c,3,(O),x,Ring,Ring1
 pyridoxamine|pyridoxamin root root
 N,x,C,4,c,x,Ring,Ring1,c,x,(,x,C,5,O,x,),x,c,6,n,1,c,2,(C),x,c,3,(O),x,Ring,Ring
 1

pyraz root root
 c,2|o|ortho,Ring,Ring1,c,3|m|meta,Ring,Ring2,.,x,n,1|n,Ring,Ring3,Ring,Ring1,.,x
 ,n,4|p|para|n',Ring,Ring2,c,5,c,6,Ring,Ring3
 pyrazino opfuser unknown
 c,2|o|ortho,Ring,Ring1,c,3|m|meta,n,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
 pyrimid root root
 c,2|o|ortho,Ring,Ring1,n,3|m|meta,c,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
 pyrimido|pyrimid opfuser unknown
 c,2|o|ortho,Ring,Ring1,n,3|m|meta,c,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
 pyridaz root root c,3,Ring,Ring1,c,4,c,5,c,6,n,1|n,n,2|n',Ring,Ring1
 pyridazo|pyridazino opfuser unknown
 c,3,Ring,Ring1,c,4,c,5,c,6,n,1|n,n,2|n',Ring,Ring1
 triazine|triazin|symtriazine|symtriazin root root
 c,2,Ring,Ring1,n,3,c,4,n,5,c,6,n,1,Ring,Ring1
 astriazine|astriazin|asymtriazine|asymtriazin root root
 n,2,Ring,Ring1,c,3,n,4,c,5,c,6,n,1,Ring,Ring1
 strioxane|stroioxan|symtrioxane|symtrioxan root root
 C,2,Ring,Ring1,O,3,C,4,O,5,C,6,O,1,Ring,Ring1
 astrioxane|astrioxan|asymtrioxane|asymtrioxan root root
 O,2,Ring,Ring1,C,3,O,4,C,5,C,6,O,1,Ring,Ring1
 strithiane|strithian|symtrithiane|symtrithian root root
 C,2,Ring,Ring1,S,3,C,4,S,5,C,6,S,1,Ring,Ring1
 astrithiane|astrithian|asymtrithiane|asymtrithian root root
 S,2,Ring,Ring1,C,3,S,4,C,5,C,6,S,1,Ring,Ring1
 triazino|symtriazino opfuser unknown
 c,2,Ring,Ring1,n,3,c,4,n,5,c,6,n,1,Ring,Ring1
 astriazino|asymtriazino opfuser unknown
 n,2,Ring,Ring1,c,3,n,4,c,5,c,6,n,1,Ring,Ring1
 strioxano|symtrioxano opfuser unknown
 C,2,Ring,Ring1,O,3,C,4,O,5,C,6,O,1,Ring,Ring1
 astrioxano|asymtrioxano opfuser unknown
 O,2,Ring,Ring1,C,3,O,4,C,5,C,6,O,1,Ring,Ring1
 strithiano|symtrithiano opfuser unknown
 C,2,Ring,Ring1,S,3,C,4,S,5,C,6,S,1,Ring,Ring1
 astrithiano|asymtrithiano opfuser unknown
 S,2,Ring,Ring1,C,3,S,4,C,5,C,6,S,1,Ring,Ring1
 borazine|borazin root root N,1,Ring,Ring1,[B],2,N,3,[B],4,N,5,[B],6,Ring,Ring1
 phosphazine|borazin root root n,2,Ring,Ring1,p,3,n,4,p,5,n,6,p,1,Ring,Ring1
 pyrrole|pyrrol root root r,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 pyrrolo|pyrrol opfuser unknown n,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 pyrrolid root root N,1,Ring,Ring1,C,2|a|alpha,C,3|b|beta,C,4,C,5,Ring,Ring1
 pyrrolidino root root N,4€1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
 imidazole|imidazol|glyoxaline|glyoxalin root root
 c,2,Ring,Ring1,n,3,c,4,=,x,c,5,n,1|prefhydro,Ring,Ring1
 imidazolo|imidazol|imidazo|imidaz opfuser unknown
 c,2,Ring,Ring1,n,3,c,4,=,x,c,5,n,1,Ring,Ring1
 imidazolid root root C,2,Ring,Ring1,N,3,C,4,C,5,N,1,Ring,Ring1
 pyrazole|pyrazol root root n,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
 pyrazolo|pyrazol opfuser unknown n,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
 tetrazolium root root n,1,Ring,Ring1,[n+],2,n,3,n,4,c,5,Ring,Ring1
 pyrazabole|pyrazabol root root
 c,1,Ring,Ring1,c,2,c,3,n,3a,n,8a,(,x,[B],8,),x,Ring,Ring1,.,x,[B],4,n,4a,Ring,Ri
 ng2,c,5,c,6,c,7,n,7a,Ring,Ring2
 isooxazole|isooxazol|isoxazole|isoxazol|isoazole|isoazol root root
 o,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
 isooxazolo|isooxazol|isoxazolo|isoxazol opfuser unknown
 o,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1

isooxazolid|isooxazolid|isoxazolid|isoxazolid|isoazolid|isoazolid root root
 O,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
 urazole|urazol root root N,1,Ring,Ring1,N,2,C,3,(=O),x,N,4,C,5,(=O),x,Ring,Ring1
 pyrazolid root root N,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
 furan|fur root root o,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,4,c,5,Ring,Ring1
 furo opfuser unknown o,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 furfur root root C,a|alpha,c,2,Ring,Ring1,c,3,c,4,c,5,o,1,Ring,Ring1
 then root root C,2,c,x,Ring,Ring1,c,3,c,4,c,5,s,1,Ring,Ring1
 furazan root root c,3,Ring,Ring1,c,4,n,5,o,1,n,2,Ring,Ring1
 isothiazole|isothiazol root root s,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
 isothiazolo|isothiazol opfuser unknown s,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
 isosulfonazole|isosulfonazol root root
 c,4,Ring,Ring1,c,5,s,1,(=,x,O,x,) (=,x,O,x,),x,n,2,c,3,Ring,Ring1
 isoselenazole|isoselenazol root root
 [se],1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
 isoselenazolo|isoselenazol opfuser unknown
 [se],1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
 benzisosulfonazole|benzisosulfonazol root root
 s,1,(=,x,O,x,) (=,x,O,x,),x,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,
 7a,Ring,Ring2,Ring,Ring1
 benzsulfonazole|benzsulfonazol root root
 s,1,(=,x,O,x,) (=,x,O,x,),x,Ring,Ring1,c,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,
 7a,Ring,Ring2,Ring,Ring1
 sulfonazole|sulfonazol root root
 s,1,(=,x,O,x,) (=,x,O,x,),x,Ring,Ring1,c,2,n,3,c,4,c,5,Ring,Ring1
 thiophene|thien root root
 c,2|a|alpha,Ring,Ring1,c,3|b|beta,c,4,c,5,s,1,Ring,Ring1
 thieno|thien opfuser unknown c,2,Ring,Ring1,c,3,c,4,c,5,s,1,Ring,Ring1
 selenophene|selenophen root root [se],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 selenopheno|selenophen opfuser unknown
 [se],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 tellurophene|tellurophen root root [Te],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 telluropheno|tellurophen opfuser unknown
 [Te],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 piperid root root N,1|n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1
 piperidino root root N,4@1|n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1
 homopiperid root root N,1|n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,Ring,Ring1
 nipecot root root C,a|alpha,C,3,Ring,Ring1,C,4,C,5,C,6,N,1|n,C,2,Ring,Ring1
 isonipecot root root C,a|alpha,C,4,Ring,Ring1,C,5,C,6,N,1|n,C,2,C,3,Ring,Ring1
 purine|purin root root
 n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,n,1,c,6,c,5,Ring,Ring1,R
 ing,Ring2
 adenine|adenin root root
 n,1,Ring,Ring1,c,2,n,3,c,4,(,x,c,5,Ring,Ring2,c,6,(,x,N,n|n6,),x,Ring,Ring1,),x,
 n,9,c,8,n,7|prefhydro,Ring,Ring2
 piperaz root root N,1|n,Ring,Ring1,C,2,C,3,N,4|n',C,5,C,6,Ring,Ring1
 piperazino root root N,4@1|n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,Ring,Ring1
 homopiperaz root root N,1|n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,C,7,Ring,Ring1
 homopiperazino root root N,4@1|n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,C,7,Ring,Ring1
 pyrroliz root root
 n,4,Ring,Ring1,Ring,Ring2,c,5,c,6,c,7,c,7a,Ring,Ring1,c,1,c,2,c,3,Ring,Ring2
 pentalene|pentalen root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring1,Ring,Ring2
 pentaleno|pentalen root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring1,Ring,Ring2

heptalene|heptalen root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,5a,Ring,Ring2,c,6,c,7,c,8,c,9,c,10,c,10a,Ring,Ring1,Ring,Ring2
 asindacene|asindacen root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,Ring,Ring3,c,8b,Ring,Ring2,Ring,Ring1
 sindacene|sindacen root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,4a,Ring,Ring3,c,5,c,6,c,7,c,7a,Ring,Ring3,c,8,c,8a,Ring,Ring2,Ring,Ring1
 octalene|octalen root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,6a,Ring,Ring2,c,7,c,8,c,9,c,10,c,11,c,12,c,12a,Ring,Ring1,Ring,Ring2
 mevalon root root C,1,C,2,C,3,(,x,C,4,C,5,O,x,) (,x,O,x,),x,C,x
 lact|lactyl root root C,1,C,2|alpha|a,(,x,O,x,),x,C,3|b|beta
 24d root root
 O,1@x,C,x,(=,x,O,x,),x,C,a|alpha,O,x,c,1,Ring,Ring1,c,2,(,x,C1,x,),x,c,3,c,4,(,x,C1,x,),x,c,5,c,6,Ring,Ring1
 245t root root
 O,1@x,C,x,(=,x,O,x,),x,C,a|alpha,O,x,c,1,Ring,Ring1,c,2,(,x,C1,x,),x,c,3,c,4,(,x,C1,x,),x,c,5,c,6,Ring,Ring1
 dnp|24dnp root root c,4@1,Ring,Ring1,c,x,([N+](=O)[O-]),x,c,3|m|meta,c,x,([N+](=O)[O-]),x,c,5,c,6,Ring,Ring1
 morphol root root C,2,Ring,Ring1,C,3,N,4,C,5,C,6,O,1,Ring,Ring1
 morpholino root root O,1,Ring,Ring1,C,2,C,3,N,4@4,C,5,C,6,Ring,Ring1
 semicarbazide|semicarbazid root root N,1,N,2,C,X,(=,x,O,3,),x,N,4
 semicarbazido root root N,4@1,N,2,C,X,(=,x,O,3,),x,N,4
 isosemicarbazide|isosemicarbazid root root N,1,N,2,C,X,(,x,O,3,) =,x,N,4
 isosemicarbazido root root N,4@1,N,2,C,X,(,x,O,3,) =,x,N,4
 semicarbazono root root N,8@1,N,2,C,X,(=,x,O,3,),x,N,4
 carbaz root root C,1,N,2,N,3
 acetone|aceton root alkane C,1|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,(=O),x,C,8,
 acetylacetone root root C,1,C,2,(=,x,O,x,),x,C,3,C,4,(=,x,O,x,),x,C,5
 isobutyron|isobutyron root root CC(C)C(=O)C(C)C,X
 isovaleron|isovaleron root root CC(C)CC(=O)CC(C)C,X
 enanthone root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(=O),x,C,10,C,11,C,12,C,13|w|omega
 pelargone root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(=O),x,C,10,C,11,C,12,C,13,C,14,C,15,
 laurone root alkane
 C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,X,(=O),x,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23|w|omega
 myristone root alkane
 C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,X,(=O),x,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27|w|omega
 palmitone root alkane
 C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,X,(=O),x,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27,C,28,C,29,C,30,C,31|w|omega
 stearone root alkane
 C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,X,(=O),x,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27,C,28,C,29,C,30,C,31,C,32,C,33,C,34,C,35|w|omega
 silatrane|silatran root root
 [Si],1,Ring,Ring1,Ring,Ring2,O,2,C,3,C,4,N,5,(,x,C,6,C,7,O,8,Ring,Ring1,),x,C,11,C,10,O,9,Ring,Ring2

glycoluril root root
 N,n|1,Ring,Ring1,C,2,(=,x,O,x,),x,N,n'|3,C,3a,Ring,Ring2,N,n''|4,C,5,(=,x,O,x,),
 x,N,n'''|6,C,6a,Ring,Ring1,Ring,Ring2
 acetylene|acetylen root root C,1,#,x,C,2
 diacetylene root root C,1,#,x,C,2,C,3,#,x,C,4
 allophan root trivial C,1,(=,x,O,x,),x,N,2,C,3,(=,x,O,x,),x,N,4
 biguanide|biguanid root root N,1,C,x,(=,x,N,2,),x,N,3,C,x,(=,x,N,4,),x,N,5
 biuret root root N,1,C,2,(=,x,O,x,),x,N,3,C,4,(=,x,O,x,),x,N,5
 carbazole|carbazone root root N,1,N,2,C,3,(=,x,O,x,),x,N,4,=,x,N,5
 carbazono root root N,4@1,N,2,C,3,(=,x,O,x,),x,N,4,=,x,N,5
 carbodiazone|carbodiazon root root N,1,=,x,N,2,C,3,(=,x,O,x,),x,N,4,=,x,N,5
 carbodiazono root root N,4@1,=,x,N,2,C,3,(=,x,O,x,),x,N,4,=,x,N,5
 carbodiimide|carbodiimid root root N,n|1,=,x,C,x,=,x,N,n'|3
 sulfurdiiimide|sulfurdimid root root N,n|1,=,x,S,x,=,x,N,n'|3
 carbonohydrazide|carbonohydrazid|carbohydrazide|carbohydrazid|carbazide|carbazid
 root root N,1,N,2,C,3,(=,x,O,x,),x,N,4,N,5
 carbonohydrazido|carbohydrazido|carbazido root root
 N,4@1,N,2,C,x,(=,x,O,x,),x,N,4,N,5
 isocarbonohydrazide|isocarbonohydrazid root root
 N,1,N,2,C,x,(,x,O,x,)=,x,N,4,N,5
 isocarbonohydrazido root root N,4@1,N,2,C,x,(,x,O,x,)=,x,N,4,N,5
 formazan root root N,1,N,2,=,x,C,3,N,4,=,x,N,5
 guanidine|guanidin root root N,1|n,C,x,(,x,N,3|n',),x,=,x,N,2|n'
 guanidino|guanido root root N,4@1,C,x,(=,x,N,2,),x,N,3
 hydanto|hydant root root C,1,C,2,N,3,C,4,(=,x,O,x,),x,N,5
 hydantoin root root
 N,1,Ring,Ring1,C,2,(=,x,O,x,),x,N,3,C,4,(=,x,O,x,),x,C,5,Ring,Ring1
 rhodanine|rhodanin root root
 S,1,Ring,Ring1,C,2,(=,x,S,x,),x,N,3,C,4,(=,x,O,x,),x,C,5,Ring,Ring1
 isourea|pseudourea root root N,1|n,=,x,C,x,(,x,O,2,),x,N,3|n'
 1isoureido root root N,4@1|n,=,x,C,x,(,x,O,o,),x,N,3|n'
 3isoureido root root N,1|n,=,x,C,x,(,x,O,o,),x,N,4@3|n'
 isothiourea root root N,1|n,=,x,C,x,(,x,S,s,),x,N,3|n'
 isothiouronium root root N,1|n,=,x,C,x,(,x,[S+],s,),x,N,3|n'
 1isothioureido root root N,4@1|n,=,x,C,x,(,x,S,s,),x,N,3|n'
 3isothioureido root root N,1|n,=,x,C,x,(,x,S,s,),x,N,4@3|n'
 isoselenourea root root N,1|n,=,x,C,x,(,x,[Se],se,),x,N,3|n'
 isoselenouronium root root N,1|n,=,x,C,x,(,x,[Se+],se,),x,N,3|n'
 1isoselenoureido root root N,4@1|n,=,x,C,x,(,x,[Se],se,),x,N,3|n'
 3isoselenoureido root root N,1|n,=,x,C,x,(,x,[Se],se,),x,N,4@3|n'
 isotellurourea root root N,1|n,=,x,C,x,(,x,[Te],te,),x,N,3|n'
 isotellurouronium root root N,1|n,=,x,C,x,(,x,[Te+],te,),x,N,3|n'
 1isotelluroureido root root N,4@1|n,=,x,C,x,(,x,[Te],te,),x,N,3|n'
 3isotelluroureido root root N,1|n,=,x,C,x,(,x,[Te],te,),x,N,4@3|n'
 glycer pseudosugar unknown x,x
 glycer root root C,1,C,2,(,x,O,a|alpha,),x,C,3,O,b|beta,
 pentaerythritol root root O,x,C,x,C,x,(,x,C,x,O,x,),x,(,x,C,x,O,x,),x,C,x,O,x
 pentaerythrityl root root C,4@x,C,x,(,x,C,4@x,),x,(,x,C,4@x,),x,C,4@x
 alphapinene root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,(,x,C,10,)=,x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
 ,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
 betapinene root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,(=,x,C,10,),x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
 ,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
 carve|carv|carvne root root
 C,2,Ring,Ring1,C,3,C,4,(,x,C,8,(=,x,C,9,),x,C,10,),x,C,5,c,6,c,1,(,x,C,7,),x,Rin
 g,Ring1

dihydrocarve|dihydrocarv|carvomenth root root
C,2,Ring,Ring1,C,3,C,4,(,x,C,8,(=,x,C,9,),x,C,10,),x,C,5,C,6,C,1,(,x,C,7,),x,Ring
 g,Ring1
 carvacr root root
c,2,Ring,Ring1,c,3,c,4,(,x,C,8,(,x,C,9,),x,C,10,),x,c,5,c,6,c,1,(,x,C,7,),x,Ring
 ,Ring1
 betaapinene root root
C,1,Ring,Ring1,Ring,Ring2,C,2,(=,x,C,10,),x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
 ,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
 pinacol root root
O,x,C,x,(,x,C,x,),x,(,x,C,x,),x,C,x,(,x,O,x,),x,(,x,C,x,),x,C,x
 pinacolyl root root
C,4@x,(,x,C,x,),x,C,x,(,x,C,x,),x,(,x,C,x,),x,C,x
 pinacolone root root
C,1,C,2,(=,x,O,x,),x,C,3,(,x,C,x,),x,(,x,C,x,),x,C,x
 benzopinacole|benzopinacol root root
C,x,(,x,C,x,(,x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,(,x,c,1',Ring,
Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2,),x,(O),x,),x,(,x,c,1'',Ring,Ring3,c,2
'',c,3'',c,4'',c,5'',c,6'',Ring,Ring3,),x,(,x,c,1''',Ring,Ring4,c,2''',c,3''',c,
4''',c,5''',c,6''',Ring,Ring4,),x,O,x
 benzopinacolone root root
O=C(C4=CC=CC=C4)C(C2=CC=CC=C2)(C3=CC=CC=C3)C1=CC=CC=C1,x
 resorcinol root root
O,o,c,1,Ring,Ring1,c,2,c,3,(,x,O,o'),,x,c,4,c,5,c,6,Ring,Ring1
 orsellin root root
c,2|o|ortho,Ring,Ring1,c,3,(,x,O,o'),,x,c,4|p|para,c,5,(,x,O,o'),,x,c,6,c,1,(C)
 ,x,Ring,Ring1
 olivetol root root
O,x,c,1,Ring,Ring1,c,2,c,3,(,x,O,x,),x,c,4,c,5,(CCCCC),x,c,6,Ring,Ring1
 hydroquinone|hydroquinon root root
c,1,Ring,Ring1,Ring,Ring2,c,2,c,3,c,4,Ring,Ring3,c,5,c,6,Ring,Ring1,,x,O,o,Ring
 ,Ring2,,x,O,o',Ring,Ring3
 syring root root
C,x,c,1,Ring,Ring1,c,2,c,3,(,x,OC,x,),x,c,4,(,x,O,x,),x,c,5,(,x,OC,x,),x,c,6,Rin
 g,Ring1
 syringol root root
O,x,c,1,Ring,Ring1,c,2,(OC),x,c,3,c,4,c,5,c,6,(OC),x,Ring,Ring1
 pyrogallol root root
O,x,c,1,Ring,Ring1,c,2,(,x,O,x,),x,c,3,(,x,O,x,),x,c,4,c,5,c,6,Ring,Ring1
 orcinol root root
O,x,c,1,Ring,Ring1,c,2,c,3,(,x,O,x,),x,c,4,c,5,(,x,C,x,),x,c,6,Ring,Ring1
 pyrogallitol root root
O,x,C,1,Ring,Ring1,C,2,(,x,O,x,),x,C,3,(,x,O,x,),x,C,4,C,5,C,6,Ring,Ring1
 phloroglucin root root
c,1,Ring,Ring1,c,2,c,3,(,x,O,x,),x,c,4,c,5,(,x,O,x,),x,c,6,Ring,Ring1
 phloroglucide root root
Oc1cc(O)c(c2cc(O)cc(O)c2)c(O)c1,x
 thym root root
c,3,Ring,Ring1,c,2,c,1,(,x,C,x,),x,c,6,c,5,c,4,(,x,C,x,(,x,C,x,),x,C,x,),x,Ring,
 Ring1
 isopuleg root root
C,x,Ring,Ring1,C,x,C,x,(,x,C,x,),x,C,x,C,x,(,x,C,x,(=,x,C,x,),x,C,x,),x,Ring
 ,Ring1
 pyrocatechol|orthocatechol root root
O,x,c,1,Ring,Ring1,c,2,(,x,O,x,),x,c,3,c,4,c,5,c,6,Ring,Ring1
 nitrone|nitron root root
C,a|alpha,=,x,[N+],n,[O-],x
 glyoxime|glyoxim root root
C,x,(,x,C,x,=,x,N,x,O,x,),x,=,x,N,x,O,x
 coumarine|coumarin|cumarin root root
o,1,Ring,Ring1,c,2,(=,x,O,x,),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
 g,Ring1,Ring,Ring2

isocoumarin|isocumarin root root
 C,1,Ring,Ring1,(=,x,O,x,),x,o,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
 g,Ring1,Ring,Ring2
 coumaran root root
 O,1,Ring,Ring1,C,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
 2
 coumarone|coumaron root root
 o,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
 2
 ayapin root root
 o,1,Ring,Ring1,c,2,(=,x,O,x,),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,(,x,COc,x,Ring,R
 ing3,),x,c,7,Ring,Ring3,c,8,c,8a,Ring,Ring1,Ring,Ring2
 benzhydr root root
 C,a|alpha,(,x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,
 c,2',c,3',c,4',c,5',c,6',Ring,Ring2
 benzoguanamine|benzoguanamin root root
 c,1,(,x,Ring,Ring1,n,2,c,3,(,x,N,x,),x,n,4,c,5,(,x,N,x,),x,n,6,Ring,Ring1,),x,c,
 1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
 trit root root
 C,a|alpha,Ring,Ring1,Ring,Ring2,Ring,Ring3,,x,c,4,Ring,Ring4,Ring,Ring5,,x,c,4
 ',Ring,Ring6,Ring,Ring7,,x,c,4'',Ring,Ring8,Ring,Ring9,,x,c,3,Ring,Ring4,c,2,c
 ,1,Ring,Ring1,c,6,c,5,Ring,Ring5,,x,c,3',Ring,Ring6,c,2',c,1',Ring,Ring2,c,6',c
 ,5',Ring,Ring7,,x,c,3'',Ring,Ring8,c,2'',c,1'',Ring,Ring3,c,6'',c,5'',Ring,Ring
 9
 ureth root root N,n,C,x,(=,x,O,x,),x,O,x,C,x,C,x
 chalcone|chalcon root root
 C,a|alpha,(,x,C,x,(=,x,O,x,),x,c,1',Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Rin
 g1,),x,=,x,C,b|beta,c,1,Ring,Ring2,c,2,c,3,c,4,c,5,c,6,Ring,Ring2
 deoxybenzoin root root
 C,a|alpha,(,x,C,x,(=O),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',
 Ring,Ring2,=,x,C,2',c,3',c,4',c,5',c,6',Ring,Ring2
 thiurammonosulfide|thiurammonosulfid root root
 N,n,C,x,(=,x,S,x,),x,S,x,C,x,(=,x,S,x,),x,N,n'
 thiuramdisulfide|thiuramdisulfid root root
 N,n,C,x,(=,x,S,x,),x,SS,x,C,x,(=,x,S,x,),x,N,n'
 thiuramtrisulfide|thiuramtrisulfid root root
 N,n,C,x,(=,x,S,x,),x,SSS,x,C,x,(=,x,S,x,),x,N,n'
 thiuramtetrasulfide|thiuramtetrasulfid root root
 N,n,C,x,(=,x,S,x,),x,SSSS,x,C,x,(=,x,S,x,),x,N,n'
 mercuran root root S=C(SSC(N(C)C)=S)N(C)C,x
 diacetamide|diacetamid root root
 N,n,(,x,C,x,(,x,=,x,O,x,),x,C,x,),x,C,x,(,x,=,x,O,x,),x,C,x
 triacetamide|triacetamid root root
 N,x,(,x,C,x,(,x,=,x,O,x,),x,C,x,),x,(,x,C,x,(,x,=,x,O,x,),x,C,x,),x,C,x,(,x,=,x,
 O,x,),x,C,x
 dibenzamide|dibenzamid root root
 N,n,(,x,C,x,(,x,=,x,O,x,),x,c,x,Ring,Ring1,ccccc,x,Ring,Ring1,),x,C,x,(,x,=,x,O
 x,),x,c,x,Ring,Ring2,ccccc,x,Ring,Ring2
 tribenzamide|tribenzamid root root
 N,x,(,x,C,x,(,x,=,x,O,x,),x,c,x,Ring,Ring1,ccccc,x,Ring,Ring1,),x,(,x,C,x,(,x,=,
 x,O,x,),x,c,x,Ring,Ring2,ccccc,x,Ring,Ring2,),x,C,x,(,x,=,x,O,x,),x,c,x,Ring,Rin
 g3,=,x,ccccc,x,Ring,Ring3
 fulvene|fulven root root
 C,6,=,x,C,5,Ring,Ring1,C,1,=,x,C,2,C,3,=,x,C,4,Ring,Ring1
 stilbene|stilben root root
 C,b|beta|a'|alpha',(=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|pa

ra,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,c,2' |o'|ortho',c,3' |m'|meta',c,4' |p'|p
 ara',c,5',c,6',Ring,Ring2
 stilbestrol|stilboestrol root root
 C,b|beta,(=,x,C,a|alpha,c,1,Ring,Ring1,c,2,c,3,c,4,(O),x,c,5,c,6,Ring,Ring1,),x,
 c,1',Ring,Ring2,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring2
 hexestrol root root
 C,b|beta,(CC),(,x,C,a|alpha,(CC),x,c,1,Ring,Ring1,c,2,c,3,c,4,(O),x,c,5,c,6,Ring,
 Ring1,),x,c,1',Ring,Ring2,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring2
 benzil root root
 C(=O),x,(,x,C(=O),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',Ring,
 Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
 antipyr|antipyrene|phenazone root root
 C,4,Ring,Ring1,C,5,(=O),x,N,1,(,x,N,2,(,x,C,x,),x,C,3,(,x,C,x,),x,=,x,Ring,Ring1
 ,),x,c,1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
 glycid root root C,1,C,2|b|beta,Ring,Ring1,C,3,O,x,Ring,Ring1
 ketene|keten root root C=C=O,1
 diketene|diketen root root C=C1CC(=O)O1,x
 adamant root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,Ring,Ring3,C,4,C,5,(,x,C,6,C,7,(,x,C,8,Ring,Ri
 ng1,),x,C,10,Ring,Ring3,),x,C,9,Ring,Ring2
 noradamant root root
 C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,Ring,Ring3,C,4,C,5,(,x,C,6,C,7,(,x,C,8,Ring,Ri
 ng1,),x,Ring,Ring3,),x,C,9,Ring,Ring2
 hexamethylenetetramine|hexamethylenetetramin root root
 N,1,Ring,Ring1,Ring,Ring2,C,2,N,3,Ring,Ring3,C,4,N,5,(,x,C,6,N,7,(,x,C,8,Ring,Ri
 ng1,),x,C,10,Ring,Ring3,),x,C,9,Ring,Ring2
 pentamethylenetetramine|pentamethylenetetramin root root N12CNCN(CNC1)C2,x
 fulvalene|fulvalen root root
 c,2,Ring,Ring1,(,x,c,3,c,4,c,5,c,1,Ring,Ring1,) =,x,c,2',Ring,Ring2,c,3',c,4',=,x
 ,c,5',c,1',Ring,Ring2
 tetrathiafulvalene|tetrathiafulvalen root root
 C,2,Ring,Ring1,(,x,S,3,C,4,=,x,C,5,S,1,Ring,Ring1,) =,x,C,2',Ring,Ring2,S,3',C,4'
 ,=,x,C,5',S,1',Ring,Ring2
 tetraselenafulvalene|tetraselenafulvalen root root
 C,2,Ring,Ring1,(,x,[Se],3,C,4,=,x,C,5,[Se],1,Ring,Ring1,) =,x,C,2',Ring,Ring2,[Se
],3',C,4',=,x,C,5',[Se],1',Ring,Ring2
 labd root natural
 C,1,Ring,Ring1,C,2,C,3,[C@@],4,(,x,C,18,),x,(,x,C,19,),x,[C@@],5,([H]),x,Ring,Ri
 ng2,C,6,C,7,[C@],8|a-r,(,x,C,17,),x,[C@@],9|a-
 b,(,x,[C@],10,Ring,Ring2,Ring,Ring1,C,20,),x,C,11|a-
 t,C,12,[C@],13,(,x,C,16,),x,C,14,C,15
 ambros root natural C,2,Ring,Ring1,C,3,C,4,[C@@],5|a-
 b,Ring,Ring2,(,x,C,15,),x,C,6|a-
 r,[C@],7,(,x,C,11,(,x,C,12,),x,C,13,),x,C,8,C,9,[C@],10,(,x,C,14,),x,[C@@],1|a-
 t,([H]),x,Ring,Ring2,Ring,Ring1
 cedr root natural [C@@],2,Ring,Ring1,(,x,C,12,),x,C,3,C,4,[C@],5|a-
 b,([H]),x,Ring,Ring2,[C@@],6|a-
 r,(,x,C,13,),x,(,x,C,14,),x,[C@],7,(,x,C,11,Ring,Ring3,),x,[C@],8,(,x,C,15,),x,C
 ,9,C,10,[C@@],1|a-t,Ring,Ring1,Ring,Ring2,Ring,Ring3
 cedrol root natural OC1(C)C3CC2(C(C3(C)C)CCC2C)CC1,x
 apotrichothec root natural
 O,1,Ring,Ring1,[C@],12,Ring,Ring2,(,x,C,13,),x,C,2,C,3,C,4,[C@@],5|a-
 r,(,x,C,14,),x,Ring,Ring2,[C@],6|a-
 b,(,x,C,15,),x,Ring,Ring3,C,7,C,8,C,9,(,x,C,16,),x,C,10,[C@],11|a-
 t,([H]),x,Ring,Ring3,Ring,Ring1

germacr root natural
C1,Ring,Ring1,C2,C3,[C@],4,(,x,C,15,),x,C5,C6,[C@],7,(,x,C,11,(,x,C,12,),x,C,13,),x,C8,C9,[C@@],10,(,x,C,14,),x,Ring,Ring1
 podocarpa|podocarp root steroid
C1,Ring,Ring1,C2,C3,[C@],4,(,x,C,15|18,),x,(,x,C,16|19,),x,C5,Ring,Ring2,C6,C7,C8,Ring,Ring3,C14,C13,C12,C11,C9,Ring,Ring3,[C@@],10,(,x,C,17,),x,Ring,Ring1,Ring,Ring2
 palustr root natural
C,x,Ring,Ring4,..,x,CC(C)C(CC3)=CC2=C3[C@]1(C)C(CC2)[C@@],x,Ring,Ring4,(C)CCC1,x
 gedun root natural
C1,Ring,Ring1,C2,C3,C4,(,x,C,30,),x,(,x,C,31,),x,C5,Ring,Ring2,C6,C7,C8,Ring,Ring3,(,x,C,x,),x,C14,Ring,Ring4,C15,C16,O,x,C17,(,x,C,20,Ring,Ring5,C,x,O,x,C,23,C22,Ring,Ring5,),x,C13,Ring,Ring4,(,x,C,18,),x,C12,C11,C9,Ring,Ring3,C10,(,x,C,19,),x,Ring,Ring2,Ring,Ring1
 eudesm root natural
C1,Ring,Ring1,C2,C3,[C@],4,(C),x,[C@@],5,([H]),x,Ring,Ring2,C6,[C@],7|a-r,(,x,C,11,(C),x,C,x,),x,C8|a-b,C9|a-t,[C@],10,(C),x,Ring,Ring2,Ring,Ring1
 trichotheca|trichothec root natural
C3,Ring,Ring1,C4,[C@@],5|a-r,(,x,C,14,),x,Ring,Ring2,[C@],6|a-
b,(,x,C,15,),x,Ring,Ring3,C7,C8,[C@],9,(,x,C,10,[C@],11|a-t,([H]),x,Ring,Ring3,O1,[C@],2,Ring,Ring1,[C@],12,Ring,Ring2,C13,),x,C16
 scirpenol root natural
[C@],3,(O),x,Ring,Ring1,C4,[C@@],5|a-r,(,x,C,14,),x,Ring,Ring2,[C@],6|a-
b,(,x,C,15,),x,Ring,Ring3,C7,C8,C9,(=,x,C,10,[C@],11,([H]),x,Ring,Ring3,O1,[C@],2,Ring,Ring1,[C@@],12,Ring,Ring2,(,x,O,x,Ring,Ring4,),x,C13,Ring,Ring4,),x,C16
 prosta|prost root natural
C1,C2,C3,C4,C5,C6,C7,[C@@H],8|a-t,(,x,C,9,C10,C11,Ring,Ring1,),x,[C@H],12|a-b,Ring,Ring1,C13|a-r,C14,C15,C16,C17,C18,C19,C20
 phorbol root natural
O,x,[C@@],13,1,(,x,[C@@H],12,2O)[C@H]([C@@](C=C,a-t,Ring,Ring3,CO)([H])[C@@](O)([C@@](C=C(C)C4=O)([H]),x,[C@],4|a-b,4(O)C,a-r,3)[C@@H]2C)[C@@]1(C)C,x
 tigli|tiglia root natural
C13,Ring,Ring1,(,x,C,12,Ring,Ring2,),x,[C@H],x,(,x,[C@@],8,(,x,C,7,=,x,C,6|a-t,Ring,Ring3,C20,),x,([H]),x,C9,(,x,[C@@],10,(,x,C,1,C2,(C),x,C,3,Ring,Ring4,),x,([H]),x,C4|a-b,Ring,Ring4,C5|a-r,Ring,Ring3,),x,[C@@H],x,Ring,Ring2,C,x,),x,[C@@],x,Ring,Ring1,(C),x,C,x
 glutathionereduced root root
O=C(NCC(,x,O,1@x,)=O)C(C,x,S,s,)NC(CCC(N)C(,x,O,1@x,)=O)=O,x
 glutathione root root
O=C(NCC(O)=O)[C@H](CSSC[C@H](NC(CC[C@H](N)C(O)=O)=O)C(NCC(O)=O)=O)NC(CC[C@H](N)C(O)=O)=O,x
 sphingosin|sphingosine|dihydrosphingosin|dihydrosphingosine pseudosugar unknown
x,x
 sphingosin|sphingosine root root
O,x,C,1,C,2,(,x,N,n,),x,C,3,(O),x,C,4,=,x,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18
 dihydrosphingosin|dihydrosphingosine root root
O,x,C,1,C,2,(,x,N,x,),x,C,3,(O),x,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18
 phenacetin root root
CCOC1=CC=C(NC(C)=O)C=C1,x
 xanthotoxin root root
COCl=C(OC3=O)C(C=C3)=CC2=C1OC=C2,x
 troxonium root root
O=C(C1=CC(OC)=C(C(OC)=C1)OC)OCC[N+](CC)(CC)CC,x
 triclopyr root root
O,1@x,C(=O)CO(N=C(C1)C(C1)=C1)=C1Cl,x
 thonzonium|tonzonium root root
COCl=CC=C(C=C1)CN(C2=NC=CC=N2)CC[N+](C)(C)CCCCCCCCCCCCCCCC,x
 tolonium root root
NC1=CC2=C(N=C(C=C3)C(S2)=CC3=[N+](C)C=C1C,x

tolazoline root root C(c1ccccc1)C2=NCCN2,x
 tiodonium root root ClC(C=C2)=CC=C2[I+]C1=CC=CS1,x
 tiemonium root root C[N+](C)(CCC(C2=CC=CC=C2)(C3=CC=CS3)O)CCOCC1,x
 tiameetonium root root CC[N+](C)(CCSCC[N+](C)(CC)C)C,x
 tibezonium root root
 CC[N+](CC)(C)CCSC2=NC1=C(N=C(C4=CC=C(C=C4)SC3=CC=CC=C3)C2)C=CC=C1,x
 tetramisole root root C1CSC2=NC(c3cccc3)CN12,x
 suxethonium root root CC[N+](C)(CCOC(CCC(OCC[N+](C)(CC)C)=O)=O)C,x
 suxamethonium|succinylcholine root root
 C[N+](C)(CCOC(CCC(OCC[N+](C)(C)C)=O)=O)C,x
 sultroponium root root C[N+](C)(C2CCC1CC(OC(C(C3=CC=CC=C3)CO)=O)C2)CCCS([O-]) (=O)=O,x
 stilonium root root CC[N+](CC)(CCOC2=CC=C(C=C2)C=CC1=CC=CC=C1)CC,x
 spiropentane root root
 C,1,Ring,Ring1,C,2,C,3,Ring,Ring1,Ring2,C,4,C,5,Ring,Ring2
 sorbitane|sorbitan root root O[C@H]([C@H]1[C@H](O)[C@H](O)CO1)CO,x
 sesamol root root OC1=CC(OCO2)=C2C=C1,x
 sepazonium root root
 C1C1=CC(C1)=C(COC(C4=CC=C(C=C4C1)C1)CN2C=C[N+](CCC3=CC=CC=C3)=C2)C=C1,x
 scopoletin root root o1c(=O)ccc2cc(OC)c(O)cc12,x
 salbutamol root root CC(C)(NCC(C1=CC(CO)=C(O)C=C1)O)C,x
 saccharin|glucarin|saccharine|glucarine root root C(=O)1NS(=O)(=O)c2cccc21,x
 saccharide|saccharinate root root C(=O)1[N-]S(=O)(=O)c2cccc21,x
 imazethapyr|pursuit root root
 O=C1NC(C2=C(C(,x,0,1@x,)=O)C=C(CC)C=N2)=NC1(C)C(C)C,x
 pyridoxine|pyridoxin root root CC1=NC=C(CO)C(CO)=C1O,x
 prolonium|hydroxytriethoium root root C[N+](C)(C)CC(O)C[N+](C)(C)C,x
 prodeconium root root CCCOC(C[N+](C)(CCOCCCCCCCCCCOCC[N+](C)(CC(OCCC)=O)C)C)=O,x
 procaine root root Nc1ccc(C(OCCN(CC)CC)=O)cc1,x
 procainamide|procaineamide root root Nc1ccc(C(NCCN(CC)CC)=O)cc1,x
 pirdonium root root CC1=CC=C(C(C3=CC=CC=C3)OCC2CCCC[N+](C)C)C=C1,x
 pentolonium|pentolinium root root C[N+](C)(CCCCC[N+](C)C)CCCC2)CCCC1,x
 lytensium|pentonium|pentamethonium root root C[N+](C)(C)CCCCC[N+](C)(C)C,x
 penoctionium root root O=C(OCC[N+](CC)(CC)CCCCCCCC)C(C2CCCC2)C1CCCC1,x
 acetaminophen|paracetamol root root O=C(NC(C=C1)=CC=C1O)C,x
 amiben|chloramben root root O,1@x,C(=O)C1=C(C1)C(N)=CC(C1)=C1,x
 chlорfenac root root O,1@x,C(=O)CC(C(C1)=CC=C1C1)=C1C1,x
 actinonin root root OCC1N(C(C(C(C)NC(C(CC(NO)=O)CCCC)=O)=O)CCC1,x
 aminopropylon root root O=C1N(c2cccc2)N(C)C(C)=C1NC(C(C)N(C)C)=O,x
 azamethonium root root CC[N+](C)(C)CCN(C)CC[N+](C)(C)CC,x
 benzathonium|benzethonium root root
 CC(C)(C1=CC=C(OCCOCC[N+](C)(C)CC2=CC=CC=C2)C=C1)CC(C)(C)C,x
 methylbenzathonium|methylbenzethonium root root
 CC(C)(C1=CC(C)=C(OCCOCC[N+](C)(C)CC2=CC=CC=C2)C=C1)CC(C)(C)C,x
 benzilonium root root O=C(OCC1C[N+](CC)(CC1)CC)C(C2=CC=CC=C2)(C3=CC=CC=C3)O,x
 bevonium root root OC(C(OCC3[N+](C)(C)CCCC3)=O)(C2=CC=CC=C2)C1=CC=CC=C1,x
 carpronium root root COC(CCC[N+](C)(C)C)=O,x
 carvone root root CC(C1=O)=CCC(C1)C(C)=C,x
 cetrimonium root root CCCCCCCCCCCCCCCC[N+](C)(C)C,x
 chloraminophen root root ClCCN(C1=CC=C(CCCC(O)=O)C=C1)CCCl,x
 chloraminophenamide root root O=S(N)(C1=C(C1)C=C(N)C(S(=O)(N)=O)=C1)=O,x
 chloramphenicol root root OC[C@H](NC(C(C1)C1)=O)[C@H](C1=CC=C([N+]([O-])=O)C=C1)O,x
 chlorphonium root root CCCC[P+](CCCC)(CCCC)CC1=CC=CC=C1,x
 ciclonium root root CC[N+](CC)(CCOC(C1CC2CC1C=C2)(C3=CC=CC=C3)C)C,x
 cyclopyrronium root root CC[N+](CCC(OC(C(C3=CC=CC=C3)C2CCCC2)=O)C1)C,x
 cypion root root CCCCC1CCCC1,x

decamethonium root root C[N+] (C) (C) CCCCCCCCCC[N+] (C) (C) C, x
 deditonium root root
 CC(C1=CC=C(C=C1OCC[N+]) (C) (CCCCCC[N+] (C) (CCOC2=CC (C)=CC=C2C (C) C) C) C) C, x
 denatonium root root CC[N+] (CC(NC(C(C)=CC=C2)=C2C)=O) (CC) CC1=CC=CC=C1, x
 dicyclopentadiene root root
 C,1,Ring,Ring1,c,2,c,3,C,3a,Ring,Ring2,C,4,Ring,Ring3,c,5,c,6,C,7,(,x,C,x,Ring,Ring3,),x,C,7a,Ring,Ring2,Ring,Ring1
 dimecolonium root root CC1CCCC([N+]1(C)C)C(OCC[N+] (C) (C) C)=O, x
 dimidium root root c1cc(N)cc2c(c3cccc3) [n+] (C)c4cc(N)ccc4c21, x
 dinoseb root root CC(C(C=C([N+] ([O-]))=O)C=C1[N+] ([O-]))=O)=C1O)CC, x
 disilethylene root root [Si],1,C,2,C,3,[Si],4
 disiquonium root root C[N+] (CCCCCC[N+] (CCC[Si] (OC) (OC) OC) CCCCCCCCCC, x
 dotefonium root root CN(C(C(C2=CC=CC=C2) (C3=CC=CS3) O)=O)CC[N+]1(CCCC1)C, x
 ebdc root root S,1@x,C(NCCNC(,x,S,1@x,)=S)=S, x
 edrophonium root root CC[N+] (C) (C1=CC=CC(O)=C1)C, x
 emepronium root root CC[N+] (C) (C(CC(C2=CC=CC=C2)C1=CC=CC=C1)C)C, x
 fentonium root root
 C[N+]3 (C4CCCC3CC(OC(C(C5=CC=CC=C5)CO)=O)C4)CC(C1=CC=C(C2=CC=CC=C2)C=C1)=O, x
 fludazonium root root
 O=C(C1=CC=C(F)C=C1)CN(C=C2)C=[N+]2CC(C4=C(C=C(C=C4)C1)C1)OCC3=C(C=C(C=C3)C1)C1, x
 furacrin loveracid root CC1=CC(C=C2C(C(CC)=C)=O)=C(C=C2C)O1, x
 fosamine|fosamin root root O=P(O) (OCC)C(N)=O, x
 fubrogonium root root CC[N+] (CC) (CCC(OC(C1=CC=C(O1)Br)=O)C)C, x
 furtrethonium root root C[N+] (C) (C)CC1=CC=CO1, x
 glufosinate|glufosinat root root CP(O) (CCC(C(,x,O,1@x,)=O)N)=O, x
 glycopyrronium root root OC(C1CCCC1) (C2=CC=CC=C2)C(OC(CC3)C[N+]3(C)C)=O, x
 glyphosate|glyphosat root root O,1@x,C(CNCP(O)(O)=O)=O, x
 heteronium root root C[N+]1(CCC(OC(C(C2=CC=CC=C2) (C3=CC=CS3)O)=O)C1)C, x
 hexafluoronium root root
 C[N+] (C) (C2C1=C(C3=C2C=CC=C3)C=CC=C1)CCCCC[N+] (C) (C6C4=C(C5=CC=CC=C56)C=CC=C4)C
 , x
 hexamethonium root root C[N+] (C) (CCCCCC[N+] (C) (C)C)C, x
 hexasonium root root C[S+] (CCOC(C(C2=CC=CC=C2)C1CCCC1)=O)C, x
 hexopyrronium root root C[N+]1(CCC(OC(C(C2CCCC2) (C3=CC=CC=C3)O)=O)C1)C, x
 imazaquin root root CC(C1(N=C(C3=NC2=CC=CC=C2C=C3C(,x,O,1@x,)=O)NC1=O)C)C, x
 isoluminol root root NC1=CC=C2C(C(NNC2=O)=O)=C1, x
 mebezonium root root C[N+] (C) (C1CCC(CC2CCC([N+] (C) (C)C)CC2)CC1)C, x
 mecetronium root root CCCCCCCCCCCCCC[N+] (C) (CC)C, x
 chloramben root root O,1@x,C(=O)C1=C(N)C(C1)=CC(C1)=C1, x
 nitronium root root O=[N+]=O, x
 nifuroxime root root ON=Cc1ccc(o1)[N+] (=O) [O-], x
 octafonium root root CC[N+] (CCOC1=CC=C(C=C1)CC(C) (CC(C)C)C) (CC2=CC=CC=C2)CC, x
 otilonium root root
 CCCCCCCCOC1=CC=CC=C1C(NC2=CC=C(C(OCC[N+] (CC) (CC)C)=O)C=C2)=O, x
 oxitefonium root root CC[N+] (CC) (CCOC(C(C1=CC=CC=C1) (C2=CC=CS2)O)=O)C, x
 pxydipentonium root root C[NH+] (CCCCCOCCCC[N+] (C) (C)C)C, x
 oxyphenonium root root CC[N+] (CC) (CCOC(C(C1CCCC1) (C2=CC=CC=C2)O)=O)C, x
 oxyppyronium root root C[N+]1(CCCC1COC(C(C2CCCC2) (C3=CC=CC=C3)O)=O)C, x
 oxysonium root root C[S+] (CCOC(C(C1CCCC1) (C2=CC=CC=C2)O)=O)C, x
 amezinium root root COC1=CC(N)=CN=[N+]1C2=CC=CC=C2, x
 amenzpyrinium root root CN(C(OC1=CC=C[N+] (CC2=CC=CC=C2)=C1)=O)C, x
 carcainium root root C[N+] (CC(NC1=CC=CC=C1)=O) (CC(NC2=CC=CC=C2)=O)C, x
 clonidine root root
 c,p,Ring,Ring1,c,m,c,x,(Cl),x,c,x,(NC2=NCCN2),x,c,x,(Cl),x,c,x,Ring,Ring1
 dequalinium root root
 CC1=CC(N)=C2C(C=CC=C2)=[N+]1CCCCCCCCC[N+] (C(C)=C3)=C(C=CC=C4)C4=C3N, x
 elliptinium root root CC(C2=C1C=C[N+] (C)=C2)=C(C3=C4C=CC(O)=C3)C(N4)=C1C, x

fazadinium root root
CC5=C(N(C6=[N+])5C=CC=C6)N=NN3C(C2=CC=CC=C2)=C([N+]4=C3C=CC=C4)C)C1=CC=CC=C1,x
 fenpiverinium root root C[N+]1(CCC(C2=CC=CC=C2)(C3=CC=CC=C3)C(N)=O)CCCCC1,x
 methanthelinium root root O=C(C2C3=C(C=CC=C3)OC1=CC=CC=C12)OCC[N+](CC)(C)CC,x
 methylthioninium root root CN(C1=CC([S+])=C(C=C(N(C)C)C=C3)C3=N2)=C2C=C1)C,x
 metocinium root root C[N+](C)(CCOC(C(C1=CC=CC=C1)(C2=CC=CC=C2)O)=O)C,x
 nicotine root root CN1C(C2=CC=CN=C2)CCC1,x
 nolinium root root C1C(C=C3)=C(C1)C=C3NC2=CC1=CC=CC=[N+]1C=C2,x
 pentolinium root root C[N+]1(CCCCCC[N+]2(C)CCCC2)CCCC1,x
 prifinium root root CC[N+]2(CCC(C2C)=C(C3=CC=CC=C3)C1=CC=CC=C1)CC,x
 promethazine root root CC(N(C)C)CN1C3=C(C=CC=C3)SC2=C1C=CC=C2,x
 pyrvinium root root
CN(C1=CC4=C([N+] (C)=C(C=C4)C=CC2=C(C)N(C3=CC=CC=C3)C(C)=C2)C=C1)C,x
 rosaniline|rosanilin root root
N=C(C=C3)C=CC3=C(C2=CC=C(N)C(C)=C2)C1=CC=C(N)C=C1,x
 senfol root root N=C=S,x
 tartrazine root root O=C1N(C3=CC=C([S](=O)([O-])=O)C=C3)N=C(C([O-])=O)C1N=NC2=CC=C([S](=O)([O-])=O)C=C2.[Na+].[Na+].x
 thonzylaminium root root COc2cc(cc2)CN(c1ncccn1)CC[N+](C)C,x
 trantelinium root root C[N+]1(C2CCC1CC(OC(C4C3=CC=CC=C3OC5=C4C=CC=C5)=O)C2)C,x
 trimethidinium root root CC1(C2CCC1(C[N+](CCC[N+](C)(C)C)(C2)C)C)C,x
 thenium root root C[N+](CCOC2=CC=CC=C2)(C)CC1=CC=CS1,x
 menrium|tropium|librium|solum root root [O-]
] [N+] (CC(NC)=N3)=C(C2=C3C=CC(C1)=C2)C1=CC=CC=C1,x
 oxapropanium root root C[N+](C)(C)CC1OCOC1,x
 furium root root [O-][N+](C1=CC=C(C2=CSC(NC(C)=O)=N2)O1)=O,x
 tropylum root root C1=CC=C[C+]C=C1,x
 acetaminophen root root Oc1ccc(cc1)NC(=O)C,x
 acetur root root CCNC(=O)C,x
 afurolol root root CC(C)(NCC(COC(C=CC=C1CO2)=C1C2=O)O)C,x
 agallol root root COCC[Hg]Cl,x
 alizarin root root O=C(c2cccc23)c1c(O)c(O)ccc1C3=O,x
 allantoin root root O=C(N1)NC(NC(N)=O)C1=O,x
 amantanum root root CCCCCCCCC[N+](C)(CCOC(C23CC1CC(C3)CC(C2)C1)=O)C,x
 aminopentamide root root CC(N(C)C)CC(C1=CC=CC=C1)(C2=CC=CC=C2)C(N)=O,x
 amprolium root root CCCC2=NC=C(C(N)=N2)C[N+]1=C(C)C=CC=C1,x
 aporph root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,C,4,C,5,N,6,(C),x,C,6a,Ring,Ring3,C,7,c,7a,Ring
 a,Ring,Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,11b,Ring,Ring1,c,11c,Ring,Ring
 2,Ring,Ring3
 noraporph root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,C,4,C,5,N,6,C,6a,Ring,Ring3,C,7,c,7a,Ring
 ,Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,11b,Ring,Ring1,c,11c,Ring,Ring2,Ring
 ,Ring3
 aspirin root root O=C(O)c1cccc1OC(C)=O,x
 azaspirium root root
COC(C1=C(C(OC)=C23)C=CO1)=C3OC5=C(C[N+]4(CC5=C)CCCC4)C2=O,x
 bephenium root root C[N+](CCOC1=CC=CC=C1)(CC2=CC=CC=C2)C,x
 berb root root c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,C,5,C,6,N,7|a-
 r,Ring,Ring3,C,8,c,8a,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,c,13|a-
 t,C,13a|a-b,Ring,Ring3,c,13b,Ring,Ring2,Ring,Ring1
 bidimazium root root
CN(C1=CC=C(C=CC2=[N+] (C)C(C3=CC=C(C4=CC=CC=C4)C=C3)=CS2)C=C1)C,x
 bretylum root root CC[N+](C)(CC1=C(Br)C=CC=C1)C,x
 busulfan root root O=S(OC(=O)COC(=O)C(=O)C)=O,x
 carazolol root root OC(CNC(C)C)COC1=CC=CC2=C1C(C=CC=C3)=C3N2,x
 clofilium root root CCCCCCCC[N+](CC)(CCCCC1=CC=C(C=C1)C1)CC,x

datelliptium root root
CC1=C4C(C=C[N+](CC[NH+]CC)=C4)=C(C)C3=C1C2=C(N3)C=CC(O)=C2,x
 demecarium root root
CN(C(OC2=CC=CC([N+]C(C)C)=C2)=O)CCCCCCCCCN(C(OC1=CC=CC([N+]C(C)C)=C1)=O)C,x
 dibromantin root root CC(C(N1Br)=O)(N(Br)C1=O)C,x
 digermin root root O=[N+]([O-])C1=CC(C(F)(F)F)=CC([N+]([O-])=O)=C1N(CCC)CCC,x
 diphenhydramine root root CN(C)CCOC(C2=CC=CC=C2)C1=CC=CC=C1,x
 dithizone root root S=C(NNC2=CC=CC=C2)N=NC1=CC=CC=C1,x
 dopamine root root
NCC,x,c,1,Ring,Ring1,c,2,c,3,(O),x,c,4,(O),x,c,5,c,6,Ring,Ring1
 etipirium root root C[N+]1(CCOC(C(C2=CC=CC=C2)(C3=CC=CC=C3)O)=O)CCCC1,x
 fench root root
C,2|a|alpha,Ring,Ring1,C,3,(C)(C),x,c,4,(,x,c,5,c,6,c,1,Ring,Ring2,(C),x,Ring,Ring1,),x,c,7,Ring,Ring2
 feniodium root root C1C2=CC=C(C(C1)=C2)[I+]C1=CC=C(C=C1C1)C1,x
 flutropium root root C[N+]1(C2CCC1CC(OC(C(C3=CC=CC=C3)(C4=CC=CC=C4)O)=O)C2)CCF,x
 furazolium root root [O-][N+](C1=CC=C(C2=CSC3=[N+]2CCN3)O1)=O,x
 halopenium root root CC(C1=CC(C1)=C(C=C1OCCC[N+]C(CC2=CC=C(C=C2)Br)C)C)C,x
 hexafluorenium root root
C[N+](C)(C2C1=C(C3=C2C=CC=C3)C=CC=C1)CCCCC[N+](C)(C6C4=C(C5=CC=CC=C56)C=CC=C4)C,x
 hexocyclium root root C[N+]1(CCN(CC(C2CCCCC2)(C3=CC=CC=C3)O)CC1)C,x
 ethidium|homidium root root
NC(C=C3)=CC2=C3C1=CC=C(N)C=C1C(C4=CC=CC=C4)=[N+]2CC,x
 indenolol root root CC(NCC(COC2=C1C=CCC1=CC=C2)O)C,x
 ionone|ionon|alphaionone root root O=C(C)C=CC1c(C)cccc1(C)C,x
 betaionone|betaionon root root O=C(C)C=CC1=C(C)cccc1(C)C,x
 isometamidium root root
CC[N+]4=C(C2=C(C5=CC=C(C=C45)N)C=CC(NN=NC3=CC=CC(C(N)=N)=C3)=C2)C1=CC=CC=C1,x
 isophor root root C,1,Ring,Ring1,C,2,c,3,(C),x,c,4,c,5,(C)(C),x,c,6,Ring,Ring1
 isophorone root root
O=,x,C,1,Ring,Ring1,C,2,=,x,C,3,(C),x,C,4,C,5,(C)(C),x,C,6,Ring,Ring1
 lapirium root root O=C(NCCOC(CCCCCC)=O)C[N+]1=CC=CC=C1,x
 methylbenactyzium root root OC(C1=CC=CC=C1)(C2=CC=CC=C2)C(OCC[N+](CC)(C)CC)=O,CC,x
 benactyzine root root CCN(CCOC(C(C1=CC=CC=C1)(C2=CC=CC=C2)O)=O)CC,x
 miripirium root root CCCCCCCCCCCC[N+]1=CC=C(C)C=C1,x
 neopentylglycol root root OCC(C)(C)CO,x
 nioxime root root ON=C(CCCC1)C1=NO,x
 oxapium root root C[N+]1(CC2COC(C3CCCCC3)(C4=CC=CC=C4)O2)CCCC1,x
 oxolin root root CC2=CN(CC)C1=CC(OCO3)=C3C=C1C2=O,x
 oxprenolol root root CC(NCC(COC1=CC=CC=C1OCC=C)O)C,x
 oxybenzone root root O=C(C1=CC=CC=C1)C(C=CC(OC)=C2)=C2O,x
 penbutolol root root OC(CNC(C)(C)C)COC1=C(C2CCCC2)C=CC=C1,x
 pentacyinium root root
C[N+](CCCCC(C1=CC=CC=C1)(C2=CC=CC=C2)C#N)(CC[N+]3(CCOC3)C)C,x
 pentazocine root root CC2C3(C)C1=CC(O)=CC=C1CC2N(CC=C(C)C)CC3,x
 phenacetur root root CCNC(=O)Cc1cccc1,x
 phencyclidine|angeldust root root c1(C2(N3CCCCC3)CCCC2)cccc1,x
 pinaverium root root COC4=CC(Br)=C(C=C4OC)C[N+]3(CCOC3)CCOCC1CCC2CC1C2(C)C,x
 piperylene root root C=CC=CC,x
 piproctanylium root root CC(C)CCCC(C)CC[N+]1(CC=C)CCCC1,x
 piprocurarium root root CC[N+]1(CC)CCOC(C([N+]2(CCCCC2)C)C1=CC=CC=C1)=O)C,x
 pranolium root root CC(C)[N+](C)(C)CC(O)COC1=C2C(C=CC=C2)=CC=C1,x
 pretamazium root root
CC[N+]3=C(SC=C3C4=CC=C(C5=CC=CC=C5)C=C4)C=CC1=CC=C(N2CCCC2)C=C1,x
 propanolol root root OC(CNC(C)C)COC1=C2C(C=CC=C2)=CC=C1,x

propidium root root
C[N+](CC)(CC)CCC[N+](C3=C2C=CC(N)=C3)=C(C4=CC=CC=C4)C1=C2C=CC(N)=C1,x
 prospidium root root C1CC(O)CN3CC[N+]2(CC3)CC[N+]1(CC2)CCN(CC1)CC(O)CC1,x
 pyritidium root root
CC1=CC(NC2=CC(C(C3=CC=C(C=C3)N)=[N+])C5=CC(N)=CC=C4)C=C4C=C2)=NC(N)=[N+]1C,x
 quinomethionate|chinomethionate root root O=C3SC2=NC1=CC(C)=CC=C1N=C2S3,x
 salicin root root O[C@H]1O[C@H](OC2=CC=CC=C2CO)[C@H](O)[C@H](O)[C@H]1O,x
 serenium root root CCOC(C=C2)=CC=C2N=NC1=CC=C(N)C=C1N,x
 sintropium root root CCCC(C(OC1CC2CCC([N+]2(C(C)C)C)C1)=O)CCC,x
 stilbazium root root
CC[N+]1=C(C=CC5=CC=C(C=C5)N4CCCC4)C=CC=C1C=CC3=CC=C(C=C3)N2CCCC2,x
 timepidium root root CCOC2CC(C[N+](C)C2)C=C(C3=CC=CS3)C1=CC=CS1,x
 tipetropium root root CCC[N+]1(C2CCC1CC(OC4C3=CC=CC=C3CSC5=CC=CC=C45)C2)C,x
 tiquizium root root C[N+]13CCCCC1CCC(C3)=C(C4=CC=CS4)C2=CC=CS2,x
 trimethylsilyldifluoride root root [Si-](C)(C)(C)(F)F,x
 tricine root root OCC(CO)(CO)NCC(O)=O,x
 toliodium root root CC2=CC=C(C=C2)[I+]C1=CC=C(C=C1)C,x
 trazium root root OC1(C4=CC=C(C=C4)C1)NC=N[N+]3=C1C2=CC=CC=C2C=C3,x
 trepirium root root C[N+](C)(CCOC(C1CCC[N+]1(C)C)=O)C,x
 tropolone|tropalone root root
O=,x,c,1,Ring,Ring1,c,7,c,6,c,5,c,4,c,3,c,2,Ring,Ring1,o,x
 tyloxapol root root NCCc1ccc(O)cc1,x
 urocan root root
C,x,C,a|alpha,=,x,C,b|beta,c,4,Ring,Ring1,n,3,c,2,n,1|prefhydro,c,5,Ring,Ring1
 verbenone root root O=C1C(C2)C(C)(C)C2C(C)=C1,x
 yohimb|yohimbin loveracid root C,x,Ring,Ring6,..,x,N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,c,5,c,6,c,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,c,21,[C@G],20,([H]),x,Ring,Ring5,C,19,C,18,[C@H],17,
(O),x,[C@H],16,Ring,Ring6,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
 yohimb|yohimba root root N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,c,5,c,6,c,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,c,21,[C@G],20,([H]),x,Ring,Ring5,C,19,C,18,C,17,C,16
,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
 yohimbine|yohimbin root root N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,c,5,c,6,c,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,c,21,[C@G],20,([H]),x,Ring,Ring5,C,19,C,18,[C@H],17,
(O),x,[C@H],16,(C(=O)OC),x,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
 oxayohimb|oxayohimba root root N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,c,5,c,6,c,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,c,21,[C@G],20,([H]),x,Ring,Ring5,C,19,C,18,O,17,C,16
,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
 morphinan root natural c,1,Ring,Ring1,c,2,c,3,c,4,c,12|a-t,Ring,Ring2,[C@],13|a-
b,Ring,Ring4,Ring,Ring3,C,5,C,6,C,7,C,8,[C@@],14,Ring,Ring3,([H]),x,[C@],9|a-
r,(,x,N,17,C,16,C,15,Ring,Ring4,),x,c,10,c,11,Ring,Ring2,Ring,Ring1
 morphine root natural
c,1,Ring,Ring1,c,2,c,3,(O),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
t,Ring,Ring2,[C@],13|a-
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,[C@@],6,(O),x,c,7,=,x,c,8,[C@@],14,Ring,R
ing3,([H]),x,[C@],9|a-
r,(,x,N,17,(C),x,c,16,C,15,Ring,Ring4,),x,c,10,c,11,Ring,Ring2,Ring,Ring1
 codeine root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
t,Ring,Ring2,[C@],13|a-

b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,[C@@],6,(O),x,C,7,=,x,C,8,[C@@],14,Ring,Ring3,([H]),x,[C@],9|a-
 r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
 codeinone root natural
 c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
 t,Ring,Ring2,[C@],13|a-
 b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(=O),x,C,7,=,x,C,8,[C@@],14,Ring,Ring3,([H]),x,[C@],9|a-
 r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
 dihydrocodeinone|hydrocodeinone root natural
 c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
 t,Ring,Ring2,[C@],13|a-
 b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(=O),x,C,7,=,x,C,8,[C@@],14,Ring,Ring3,([H]),x,[C@],9|a-
 r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
 thebacon root natural
 c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
 t,Ring,Ring2,[C@],13|a-
 b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(OC(=O)C),x,=,x,C,7,C,8,[C@@],14,Ring,Ring3,([H]),x,[C@],9|a-
 r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
 ergoline|ergolin root natural
 n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H]),x,Ring,Ring3,N,6,C,7,C,8|a-
 t,C,9|a-b,C,10|a-
 r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring,Ring4
 lyserg root natural
 C,x,Ring,Ring5,.,x,n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H]),x,Ring,Ring3,N,6,(C),x,C,7,[C@],8|a-t,Ring,Ring5,C,9|a-b,=,x,C,10|a-
 r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring,Ring4
 lysergide root natural
 C,x,Ring,Ring5,(=O)N(CC)CC.,x,n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H])
 ,x,Ring,Ring3,N,6,(C),x,C,7,[C@],8|a-t,Ring,Ring5,C,9|a-b,=,x,C,10|a-
 r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring,Ring4
 ergotaman root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 l,Ring,Ring3,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
 Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,N,x,[
 C@],2',Ring,Ring5,C,3',N,4',Ring,Ring6,C,5',C,6',N,7',Ring,Ring7,C,8',C,9',C,10'
 ,[C@],11',([H]),x,Ring,Ring7,[C@@H],12',Ring,Ring6,O,1',Ring,Ring5
 ergocornine|ergocornin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 l,Ring,Ring3,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
 Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
 x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C)
 ,x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@]
 ,12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergocornininine|ergocorninin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 l,Ring,Ring3,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
 Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O)
 ,x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C)
 ,x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@]
 ,12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergocristine|ergocristin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 l,Ring,Ring3,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
 Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
 x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(Cc9ccc

cc9),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',[H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergocryptine|ergocryptin|ergocryptine|ergocryptin|alphaergocryptine|alphaergocryptine|alphaergocryptine|alphaergocryptine|alphaergocryptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',[H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 betaergocryptine|betaergocryptin|betaergocryptine|betaergocryptin|bergocryptine|bergocryptin|bergocryptine|bergocryptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)CC),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',[H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergocryptinin|ergocryptinin|ergocryptinin|ergocryptinin|alphaergocryptinin|alphaergocryptinin|alphaergocryptinin|alphaergocryptinin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',[H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 betaergocryptinin|betaergocryptinin|betaergocryptinin|betaergocryptinin|bergocryptinin|bergocryptinin|bergocryptinin|bergocryptinin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',[H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergosine|ergosin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',[H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergotamine|ergotamin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(Cc9cccc9),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',[H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 bromocryptine|bromocryptin|bromocryptine|bromocryptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,(Br),x,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',[H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ecgonidine|ecgonidin root root
 [C@@],x,([H]),x,Ring,Ring1,Ring,Ring2,C,x,c,x,c,x,(x,C,x,(=O),x,O,1@x,),x,[C@],x,([H]),x,(x,N,x,(C),x,Ring,Ring1,),x,C,x,C,x,Ring,Ring2

ecgonine|ecgonin root root
[C@H],x,([H]),x,Ring,Ring1,Ring,Ring2,C,x,[C@H],x,(O),x,[C@H],x,(,x,C,x,(=O),x,O,1@x,),x,[C@H],x,(,x,N,x,(C),x,Ring,Ring1,),x,C,x,C,x,Ring,Ring2
 methylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(C),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,c,2',c,3',[n+],4',(C),x,c,5',c,6',Ring,Ring2
 ethylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(CC),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,c,2',c,3',[n+],4',(CC),x,c,5',c,6',Ring,Ring2
 benzylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(Cc3cccc3),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,c,2',c,3',[n+],4',(Cc4cccc4),x,c,5',c,6',Ring,Ring2
 pheneturide root root O=C(N)NC(C(CC)C1=CC=CC=C1)=O,x
 lactide|dilactide root root CC(OC1=O)C(OC1C)=O,x
 gallion root root OC(C(Cl)=CC([N+]([O-])=O)=C3N=NC1=C(S(=O)(O)=O)C=C(C=C(S(=O)(O)=O)C=C2N)C2=C1O,x
 clofibr root root CC(C)(OC1=CC=C(C=C1)C1)C,x
 paraben root root O,1@x,C(C1=CC=C(O)C=C1)=O,x
 edetate|versenate|edta root root
O,1@x,C(CN(CC,,x,O,1@x,)=O)CCN(CC,,x,O,1@x,)=O)CC,,x,O,1@x,)=O,x
 fusar root root CC1=CC=C(CCCC)C=N1,x
 lironion root root COC1=CC=C(OC2=CC=C(C=C2)NC(N(C)C)=O)C=C1,x
 thionalide root root O=C(CS)NC2=CC1=CC=CC=C1C=C2,x
 tolperisone root root CC(C(C2=CC=C(C)C=C2)=O)CN1CCCCC1,x
 valethamate root root CCC(C(C(OCC[N+](CC)(CC)C)=O)C1=CC=CC=C1)C,x
 secbutabarital|butalan root root O=C(N1)NC(C(C(C)CC)(CC)C1=O)=O,x
 furalan root root O=C(N2)N(CC2=O)N=CC1=CC=C([N+]([O-])=O)O1,x
 boc|tboc root nprotect C,4@x,(=O)OC(C)(C)C,x
 z-nprot root nprotect C,4@x,(=O)OCc1cccc1,x
 msoc root nprotect C,4@x,(=O)OCCS(=O)(=O)C,x
 cbz root nprotect
C,4@x,(=O)OC,x,C,1,Ring,Ring1,=,x,C,2,C,3,=,x,C,4,C,5,=,x,C,6,Ring,Ring1
 fmoc root nprotect C,4@x,(=O)OCC1C2=CC=CC=C(C3=CC=CC=C13)2,x
 dansyl root nprotect S,4@x,(C2=CC=CC1=C(N(C)C)C=CC=C12)(=O)=O,x
 dabsyl root nprotect S,4@x,(c1ccc(N=Nc2ccc(N(C)C)cc2)cc1)(=O)=O,x
 bansyl root nprotect S,4@x,(C2=CC=CC1=C(N(CCCC)CCCC)C=CC=C12)(=O)=O,x
 nps root nprotect S,4@x,c1c([N+] (=O)[O-])cccc1,x
 tfa root nprotect C,4@x,(=O)C(F)(F)F,x
 acm root nprotect C,4@x,NC(=O)C,x
 phacm root nprotect C,4@x,NC(=O)Cc1cccc1,x
 creatine root root CN(C(N)=N)CC(O)=O,x
 panthenol root root CC(CO)(C(C(NCCCO)=O)O)C,x
 alanate root root [AlH4-],x
 cyanamide root root NC#N,x
 eprolin root root CC1=C2C(OC(CCCC(C)CCCC(C)CC2)=C(C)C(C)=C1O,x
 eserine|physostigmine root root O=C(NC)OC1=CC=C(N(C)C3C2(C)CCN3C)C2=C1,x
 prolan root root CC([N+]([O-])=O)C(C2=CC=C(C1)C=C2)C1=CC=C(C1)C=C1,x
 tropanserin root root CN1C2CC1CC(OC(C3=CC(C)=CC(C)=C3)=O)C2,x
 butanserin root root FC1=CC=C(C(C4CCN(CC4)CCCN3C(NC2=CC=CC=C2C3=O)=O)=O)C=C1,x
 amiprol|domalium|kiatrium|levium|relanium|tensium|umbrium|velium|valium root
 root O=C1CN=C(C3=CC=CC=C3)C2=C(C=CC(C1)=C2)N1C,x
 prolate root root S=P(OC)(OC)SCN1C(C(C=CC=C2)=C2C1=O)=O,x
 adaprolol root root CC(NCC(COC4=CC=C(C=C4)CC(OCOC23CC1CC(C3)CC(C2)C1)=O)O)C,x
 agmatine root root NC(NCCCCN)=N,x
 algolysin root root CCC(C(C1=CC=CC=C1)(C2=CC=CC=C2)CC(C)N(C)C)=O.[H]Cl,x
 altanserin root root FC1=CC=C(C(C2CCN(CCN4C(NC3=CC=CC=C3C4=O)=S)CC2)=O)C=C1,x

angelicin root root
 c,1,Ring,Ring1,c,2,o,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,(=O),
 x,o,9,c,9a,Ring,Ring3,c,9b,Ring,Ring2,Ring,Ring1
 asparaguse root root OC(C1CSSC1)=O,x
 aspartame root root O=C(OC)C(NC(C(N)CC(O)=O)=O)CC1=CC=CC=C1,x
 bisoprolol root root OC(CNC(C)C)COCl=CC=C(COCCOC(C)C)C=C1,x
 bornaprolool root root OC(CN(CC)C)CC1=CC=CC=C1C2C3CCC(C3)C2,x
 broncholysin root root OC(C(CS)NC(C)=O)=O,x
 bunaprolast root root CCCCCC2=C(OC(C)=O)C1=CC=CC=C1C(OC)=C2,x
 butethal root root CCCCC(C(NC1=O)=O)(C(N1)=O)CC,x
 capsaicin root root O=C(CCCC/C=C/C(C)C)NCC1ccc(O)c(OC)c1,x
 carbachol root root C[N+](C)(C)CCOC(N)=O,x
 carlsoprol root root CC(COC(N)=O)(CCC)CO(CNC(C)C)=O,x
 caryolysine root root ClCCN(C)CCl,x
 chloral root root O=CC(C1)(C1)C1,x
 chloralhydrate root root OC(O)C(C1)(C1)C1,x
 bromal root root O=CC(Br)(Br)Br,x
 bromalhydrate root root OC(O)C(Br)(Br)Br,x
 chrysanthemum|chrysanthem root root C1C(C=C(C)C)C(C)(C)1,x
 celiprolol root root OC(CNC(C)(C)C)COCl=C(C(C)=O)C=C(NC(N(CC)CC)=O)C=C1,x
 cinanserin root root CN(CCCSC1=CC=CC=C1NC(C=CC2=CC=CC=C2)=O)C,x
 clemepron root root CN(CC(C(C2=CC=CC(C1)=C2)C1=CC=CC=C1)O)C,x
 coumal root root Cc1ccc(=O)oc1,x
 creatinine root root N1C(=N)N(C)CC(=O)1,x
 cyclen root root
 N,1,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,N,7,C,8,C,9,N,10,C,11,C,12,Ring,Ring1
 cyprolidol root root OC(C3=CC=CC=C3)(C4=CC=CC=C4)C1CC1C2=CC=NC=C2,x
 deprol root root CC(COC(N)=O)(CCC)CO(C(N)=O)=O,x
 dibuprol root root CCCCCOCC(O)COCCCC,x
 eburnamonine root root O=C2N(c3cccc34)C1=C4CCN5C1C(CCC5)(CC)C2,x
 exaprolol root root CC(NCC(COC1=CC=CC=C1C2CCCCC2)O)C,x
 epichlorohydrin root root ClCC1CO1,x
 epithiochlorohydrin root root ClCC1CS1,x
 epifluorohydrin root root FCC1CO1,x
 epibromohydrin root root BrCC1CO1,x
 erban root root O=C(CC)NC1=CC(C1)=C(C1)C=C1,x
 ethacryl root root CCOC1=C(C1)C(C1)=C(C=C1)C(C(CC)=C)=O,x
 farmiserina|cycloserine|cycloserin|micoserina root root NC(CON1)C1=O,x
 fascaplysin root root O=C(C5=C4C=CC=C5)C1=[N+]4C=CC2=C1NC3=C2C=CC=C3,x
 febuprol root root CCCCCOCC(O)COCl=CC=CC=C1,x
 fermine root root O=C(OC)C1=CC=CC=C1C(OC)=O,x
 fertilysin root root O=C(C(C1)C1)NCCCCCCCCNC(C(C1)C1)=O,x
 formamidinedisulfide root root NC(SSC(N)=N)=N,x
 ftorafur root root O=C(N1)N(C2CCCO2)C=C(F)C1=O,x
 geneserine|eseridine root root CC23C1=CC(OC(NC)=O)=CC=C1N(C)C2ON(CC3)C,x
 glutim|pidol root root C,x,C,5,Ring,Ring1,C,4,C,3,C,2,(=O),x,N,1,Ring,Ring1
 hexethal root root O=C(N1)NC(C(CCCCCC)(CC)C1=O)=O,x
 ibuprofen root root C(C)(C)Cc1ccc(cc1)C(C)C(=O)O,x
 indameth root root ClC(C=C3)=CC=C3C(N2C(C)=C(CC(O)=O)C1=CC(OC)=CC=C12)=O,x
 iomeprol root root CN(C1=C(I)C(C(NCC(CO)O)=O)=C(I)C(C(NCC(CO)O)=O)=C1I)C(CO)=O,x
 iridocin root root NC(C1=CC(CC)=NC=C1)=S,x
 isatoicanhydride root root
 O=C(O2)c,1,Ring,Ring1,c,6,c,5,c,4,c,3,c,2,Ring,Ring1,NC2=O,x
 isoprene root root C=CC(=C)C,x
 isoxaprolool root root CC1=NOC(C=CC2=CC=CC=C2OCC(CNC(C)(C)C)O)=C1,x
 ketanserin root root FC1=CC=C(C(C2CCN(CCN4C(NC3=CC=CC=C3C4=O)=O)CC2)=O)C=C1,x

limonene root root
 C,7,c,1,Ring,Ring1,c,2,C,3,C,4,(,x,C,8,(=,x,C,9,),x,C,10,),x,C,5,C,6,Ring,Ring1
 meprol|meproleaf root root CC(COC(N)=O)(CCC)CO(N)=O,x
 metoprolol root root COCCC1=CC=C(OCC(O)CNC(C)C)C=C1,x
 mianserin root root CN1CCN3C(C2=C(CC4=CC=CC=C34)C=CC=C2)C1,x
 moprolol root root COC(C=CC=C1)=C1OCC(CNC(C)C)O,x
 myrtan root root CC1CCC(C2)C(C)(C)C21,x
 myrten root root CC1=CCC(C2)C(C)(C)C21,x
 nicainoprol root root CC(NCC(COC1=CC=CC2=C1N(C(C3=CC=CN=C3)=O)CCC2)O)C,x
 nitrogendioxide root root O,x,=,x,[N+],16@x,[O-],x
 nitricoxide root root N,32@x,=O,x
 nitrousoxide root root N#[N+] [O-],x
 ozone|trioxygen root root O=[O+] [O-],x
 oxaceprol root root CC(N1CC(CC1C(O)=O)O)=O,x
 pelanserin root root O=C2NC1=CC=CC=C1C(N2CCCN3CCN(C4=CC=CC=C4)CC3)=O,x
 phencyclone root root O=c(c(c5c3c4cccccc4c6cccccc56)c2cccccc2)c3c1cccccc1,x
 phenindione root root O=C(C2=C1C=CC=C2)C(C3=CC=CC=C3)C1=O,x
 propranolol root root OC(CNC(C)C)C0c1cccc2cccccc12,x
 psoralen root root
 o,1,Ring,Ring1,c,2,(=O),x,c,3,c,4,c,x,Ring,Ring2,c,5,c,x,Ring,Ring3,c,4',c,5',o,
 x,c,x,Ring,Ring3,c,8|8',c,x,Ring,Ring2,Ring,Ring1
 thioct root root CCCCCC1SSCC1,x
 phosphoramide|phosphorustriamide root root P(=O),x,(,x,N,n,) (,x,N,n'),x,N,n''
 pyrophosphoramide|diphosphoramide root root
 P(=O),x,(,x,N,n,) (,x,N,n'),x,O,x,P(=O),x,(,x,N,n'''),x,N,n'''
 prolintane root root CCCC(N2CCCC2)CC1=CC=CC=C1,x
 resorufin root root
 c,7,Ring,Ring1,c,6,c,5a,Ring,Ring2,o,5,c,4a,Ring,Ring3,c,4,c,3,(=O),x,c,2,c,1,c,
 10a,Ring,Ring3,n,10,c,9a,Ring,Ring2,c,9,c,8,Ring,Ring1
 retin root root
 C,15,C,14,=,x,C,13,(,x,C,20,),x,C,12,=,x,C,11,C,10,=,x,C,9,(,x,C,19,),x,C,8,=,x,
 C,7,C,6,Ring,Ring1,=,x,C,5,(,x,C,18,),x,C,4,C,3,C,2,C,1,(,x,C,16,) (,x,C,17,),x,R
 ing,Ring1
 ritanserin root root
 CC(N=C1SC=CN12)=C(CCN3CCC(CC3)=C(C5=CC=C(C=C5)F)C4=CC=C(C=C4)F)C2=O,x
 seganserin root root
 CC(NC1=CC=CC=[N]12)=C(CCN3CCC(CC3)=C(C5=CC=C(C=C5)F)C4=CC=C(C=C4)F)C2=O,x
 vinylsulfurol root root C=CC1=C(C)N=CS1,x
 teoprolol root root
 CC(NCC(COC3=CC=C3C=C(C)N4)O)CCN1C=NC(N(C(N2C)=O)C)=C1C2=O,x
 terbuprol root root COCC(COC(C)(C)C)O,x
 thyropropion aminoacid ine
 C,x,C,a|alpha,C,b|beta,C,1,Ring,Ring2,=,x,C,2|ortho,C,3|m|meta,=,x,C,4,(,x,O,x,C
 ,1',Ring,Ring3,=,x,C,2',C,3',=,x,C,4',(,x,O,x,),x,C,5',=,x,C,6',Ring,Ring3,),x,C
 ,5,=,x,C,6,Ring,Ring2
 thyroacet aminoacid ine
 C,x,C,a|alpha,C,1,Ring,Ring2,=,x,C,2|ortho,C,3|m|meta,=,x,C,4,(,x,O,x,C,1',Ring,
 Ring3,=,x,C,2',C,3',=,x,C,4',(,x,O,x,),x,C,5',=,x,C,6',Ring,Ring3,),x,C,5,=,x,C
 ,6,Ring,Ring2
 toliprolol root root CC(NCC(COC1=CC=CC(C)=C1)O)C,x
 tolysin root root O=C(C1=C3C(C=CC(C)=C3)=NC(C2=CC=CC=C2)=C1)OCC,x
 tomoxiprole root root COC1=CC=C(C4=NC2=C(N4C(C)C)C=CC3=CC=CC=C23)C=C1,x
 tricyclene|tricyclen root root CC12C(C2C3)CC3C1(C)C,x
 triprolidine root root CC1=CC=C(C(C3=NC=CC=C3)=CCN2CCCC2)C=C1,x
 tranexam root root C[C@H]1CC[C@H](CN)CC1,x
 tropicamide root root OCC(C(N(CC)CC2=CC=NC=C2)=O)C1=CC=CC=C1,x
 zipuprolol root root COC(C3=CC=CC=C3)CN1CCN(CC(C(C2=CC=CC=C2)OC)O)CC1,x

thioindigo root root O=C1C4=C(C=CC=C4)SC1=C2SC(C=CC=C3)=C3C2=O,x
 theophyllol root root O=C1C2=C(NC=N2)N(C)C(N1C)=O.O=C([O-])C.[Na+],x
 synephrine root root OC1=CC=C(C(O)CNC)C=C1,x
 sulfathiazole root root NC1=CC=C(S(NC2=NC=CS2)(=O)=O)C=C1,x
 sulfadiazine root root
 O=S(N,x,c,2,Ring,Ring1,n,3,c,4,c,5,c,6,n,1,Ring,Ring1,) (C2=CC=C(N)C=C2)=O,x
 strychnine root root O=C(C5)N(C4C2(CC7)C(N7C6)CC3C6=CCOC5C34)C1=C2C=CC=C1,x
 squalane root root CC(CCCCC(C)CCCC(C)CCCC(C)C)CCCC(C)CCCC(C)C,x
 squalene root root CC(C)=CCC\CC(C)=C\CC\CC(C)=C\CC\CC(C)=C(C)\CC/C=C(CCC=C(C)C)/C,x
 spermine|neuridine|musculamine|gerontine root root NCCCCNCCCCNCCCN,x
 spermidine root root NCCCCNCCCCN,x
 scopolamine root root CN1C2CC(OC(C(CO)c4cccc4)=O)CC1C3C2O3,x
 genoscopolamine root root C[N+]([O-])1C2CC(OC(C(CO)C4=CC=CC=C4)=O)CC1C3C2O3,x
 sendachromeal root root O=C(C(C(O)=O)=C2)C=CC2=C(C)C1=CC(C(O)=O)=C(O)C=C1,x
 sorb root root C,1,C,2,=,x,C,3,C,4,=,x,C,5,C,6
 quercitin root root OC1=CC(C(O3)=C(O)C(C2=C3C=C(O)C=C2O)=O)=CC=C1O,x
 pulegone root root CC1CC(=O)C(=C(C)C)CC1,x
 benzindopyrine|benzindopyrin root root c(CCc2ccncc2)(cn3Cc4cccc4)c1c3cccc1,x
 benziodarone|benziodaron root root O=C(c3cc(I)c(O)c(I)c3)c2c1cccc1oc2CC,x
 benzopyrronium root root C[N+](CCC(OC(C(c2cccc2)(c3cccc3)O)=O)C1)C,x
 benzothiozane|benzothiozan root root O=C(C)Nc1ccc(C=NNC(N)=S)cc1,x
 benzpiperylone|benzpiperylon root root
 O=C1C(Cc3cccc3)=C(c4cccc4)NN1C2CCN(C)CC2,x
 benzpyrinium root root CN(C(Oc1c[n+] (Cc2cccc2)ccc1)=O)C,x
 benzquinamide|benzquinamid root root
 CCN(C(C3CN2CCc1c(C2CC3OC(C)=O)cc(OC)c(OC)c1)=O)CC,x
 benzthiazide|benzthiazid root root
 O=S2(c1cc(S(N)(=O)=O)c(C1)cc1N=C(CSCc3cccc3)N2)=O,x
 benzthiazuron root root O=C(NC)Nc2sc1cccc1n2,x
 methabenzthiazuron root root O=C(NC)N(C)c2sc1cccc1n2,x
 benzvalene|benzvalen root root C13C=CC2C1C23,x
 abscis|absciss root root
 C,1,C,2,=,x,C,3,(C),x,C,4,=,x,C,5,C,6,(C(C)(C1)C)(C(C)=CC1=O)O,x
 mobenzoxamine|mabenzoxamin root root
 COc1ccc(C(c4cccc4)OCCN3CCN(CC3)CCCC(c2ccc(F)cc2)=O)cc1,x
 quinuclidine|quinuclidin root root
 N,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,C,8,Ring,Ri
 ng2
 uranine root root O=C3C=CC2=C(C4=CC=CC=C4C([O-])=O)C1=CC=C([O-
])C=C1CC2=C3.[Na+]. [Na+],x
 thorin root root OC1=C(N=NC3=C([As](O)(O)=O)C=CC=C3)C2=C(C=C(S([O-
]) (=O)C=C2)C=C1S([O-])(=O)=O.[Na+].[Na+],x
 furaneol root root CC1OC(C)=C(O)C1=O,x
 bicine|bacin root root O=C(O)CN(CCO)CCO,x
 indanthrone root root
 O=C(C3=C2C=CC=C3)C1=C(NC4=CC=C(C6=O)C(C(C7=CC=CC=C67)=O)=C4N5)C5=CC=C1C2=O,x
 methone|dimedone root root
 C,1,(=O),x,Ring,Ring1,C,2,C,3,(=O),x,C,4,C,5,(C)(C),x,C,6,Ring,Ring1
 acrinol root root NC1=C(C=C(OCC)C=C3)C3=NC2=C1C=CC(N)=C2.CC(O)C(O)=O,x
 danthron root root O=C(C2=C1C=CC=C2O)C(C(O)=CC=C3)=C3C1=O,x
 caffeine|caffein root root O=C(N(C)C2=C1N(C)C=N2)N(C)C1=O,x
 betahistine root root CNCCc1cccc1,x
 pyranine root root [O-]S(C(C=C4O)=C1C=CC2=C(S([O-])(=O)=O)C=C(S([O-
]) (=O)C3=CC=C4C1=C23)(=O)=O.[Na+].[Na+],x
 abiet root root C,x,[C@],a-
 r,2(C)C1[C@H]([C@H](CCc(C(C)C)c3)([H])C3=CC1)(C,x,C,a-t,C,a-b,2)C,x

betulin loveracid root
C[C@H]45CC[C@H]3(C)[C@]2(C)CC[C@H]1([H])C(C)(C)[C@H](O)CC[C@]1(C)[C@H]2([H])CCC
3[C@H]4([H])[C@H](C(C)=C)CC5,x
 betulin root root
OC[C@H]45CC[C@H]3(C)[C@]2(C)CC[C@H]1([H])C(C)(C)[C@H](O)CC[C@]1(C)[C@H]2([H])CC
C3[C@H]4([H])[C@H](C(C)=C)CC5,x
 caluros root root CC(C)(c1ccccc1)CC=C(C)C,x
 thymine|thymin|uracil|orot|isoorot|cytosine|isocytosine|guanine|xanthine|hypoxyan
 thine pseudosugar unknown x,x
 thymine|thymin root root
N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,(=O),x,c,5,(C),x,c,6,Ring,Ring1
 uracil root root N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,(=O),x,c,5,c,6,Ring,Ring1
 orot root root C,x,c,6,Ring,Ring1,N,1,C,2,(=O),x,N,3,C,4,(=O),x,c,5,Ring,Ring1
 isoorot root root
C,x,c,5,Ring,Ring1,c,6,n,1,c,2,(=O),x,n,3,c,4,(=O),x,Ring,Ring1
 cytosine root root
n,1|prefhydro,Ring,Ring1,c,2,(=O),x,n,3,c,4,(N),n,c,5,c,6,Ring,Ring1
 isocytosine root root
n,1|prefhydro,Ring,Ring1,c,2,(N),x,n,3,c,4,(=O),n,c,5,c,6,Ring,Ring1
 guanine pseudosugar unknown x,x
 guanine root root
n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,(N),n,N,1,c,6,(=O),x,c,5
,Ring,Ring1,Ring,Ring2
 xanthine root root
n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,(=O),x,n,1,c,6,(=O),x,c,
5,Ring,Ring1,Ring,Ring2
 hypoxyanthine root root
n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,n,1,c,6,(O),x,c,5,Ring,R
ing1,Ring,Ring2
 theophylline|theophyllin|aminophylline|aminophyllin root root
n,7,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,(C),x,c,2,(=O),x,n,1,(C),x,c,6,(=O),x,
c,5,Ring,Ring1,Ring,Ring2
 theobromine|theobromin root root
n,7,Ring,Ring1,(C),x,c,8,n,9,c,4,Ring,Ring2,n,3,(C),x,c,2,(=O),x,n,1,c,6,(=O),x,
c,5,Ring,Ring1,Ring,Ring2
 xanthopterin root root Oc1nc(N)nc2c1nc(O)cn2,x
 isoxanthopterin root root O=C1C(N=CC2=O)=C(N2)NC(N)=N1,x
 xanthopterid root root
n,1,Ring,Ring1,c,2,(N),x,n,3,c,4,(O),x,c,4a,Ring,Ring2,n,5,c,6,(O),x,c,7,n,8,c,8
a,Ring,Ring1,Ring,Ring2
 pterin|pterine root root
n,1,Ring,Ring1,c,2,(N),x,N,3,C,4,(=O),x,c,4a,Ring,Ring2,n,5,c,6,c,7,n,8,c,8a,Rin
g,Ring2,Ring,Ring1
 aminopterin root root
O,1@x,C(CCC(C(O)=O)NC(C3=CC=C(C=C3)NCC1=CN=C2C(C(N)=NC(N)=N2)=N1)=O)=O,x
 vitaminh root root O=C(N2)NC1C2CS[C@H]1CCCCC(O)=O,x
 brucine root root
O=C(C5)N(C4[C@H]2(CC7)[C@](N7C6)([H])C[C@H]3([H])C6=CCOC5[C@]34[H])C1=C2C=C(OC)C
(OC)=C1,x
 struchnine root root
O=C(C5)N(C4[C@H]2(CC7)[C@](N7C6)([H])C[C@H]3([H])C6=CCOC5[C@]34[H])C1=C2C=,x,C,1
0,C,11,=C1,x
 penicillan root root
C,x,[C@H],3,Ring,Ring2,N,4,Ring,Ring1,C,5,(,x,[C@H],6,([H]),x,[C@H],6a,Ring,Rin
g1,([H]),x,S,1,C,2,Ring,Ring2,(C)C=O,x

cephalosporan root root
 C,x,C,4,Ring,Ring1,=,x,C,3,(OOC(C)=O),x,C,2,S,1,[C@H],7a,(,x,[C@H],7,Ring,Ring2,
 [H],x,),x,([H]),x,N,5,Ring,Ring1,C,6,Ring,Ring2,=O,x
 vitaminb1|thiamine|thiamin|thiaminechloride|thiaminchlorid root root
 O3.NC1=C(C[N+]=C2=CSC(CC3)=C2C)C=NC(C)=N1.[Cl-],x
 vitaminb1nitrate|thiaminenitrate|thiaminnitrate root root
 O3.NC1=C(C[N+]=C2=CSC(CC3)=C2C)C=NC(C)=N1.[O-][N+](O-)=O,x
 thiaminedisulfide root root
 CC(N(C=O)CC1=CN=C(N=C1N)C)=C(SSC(CCO)=C(N(C=O)CC2=C(N)N=C(C)N=C2)C)CCO,x
 vitaminb2|riboflavin root root
 CC1=CC2=C(N=C(C(N3)=O)C(N2C[C@H](O)[C@H](O)[C@H](O),x,c,5',O)=NC3=O)C=C1C,x
 vitamine|alphatocopherol|atocopherol root root
 CC1=C2C(O[C@H](CCC[C@H](C)CCC[C@H](C)C(C)CC2)=C(C)C(C)=C1O,x
 phenolsulfonphthalein|phenolsulfonephthalein root root
 C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',c,4',(,x,O,x,),x,c,5',c,6',Ring,
 Ring3,),x,c,1'',Ring,Ring4,c,2',c,3',c,4',(,x,O,x,),x,c,5',c,6',Ring,Ring4
 mresolsulfonphthalein|mresolsulfonephthalein root root
 C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(,x,C,x,),x,c,5',c,
 6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2',c,3',c,4',(,x,C,x,),x,c,5',c,6',Ring,Ring4
 cresolsulfonphthalein|cresolsulfonephthalein root root
 C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(,x,C,x,),x,c,5',c,
 6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2',c,3',c,4',(,x,C,x,),x,c,5',c,6',Ring,Ring4
 pyrocatecholsulfonphthalein|pyrocatecholsulfonephthalein root root
 C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(,x,O,x,),x,c,5',c,
 6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2',c,3',c,4',(,x,O,x,),x,c,5',c,6',Ring,Ring4
 pyrogallolsulfonphthalein|pyrogallolsulfonephthalein root root
 C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(,x,O,x,),x,c,3',(O),x,c,4',(,x,O,x,),
 x,c,5',c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2',(,x,O,x,),x,c,3',(O),x,c,4',(,x,O,x,),
 x,c,5',c,6',Ring,Ring4
 thymolsulfonphthalein|thymolsulfonephthalein root root
 C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(,x,C(C)C,x,),x,c,3',c,4',(,x,O,x,),
 x,c,5',(C),x,c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2',(,x,C(C)C,x,),x,c,3',c,4',(,x,O,x,),
 x,c,5',(C),x,c,6',Ring,Ring4
 phenolphthalein root root
 C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,
 Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',c,4',(,x,O,x,),x,c,5',c,6',Ring,Ring3,),
 x,c,1'',Ring,Ring4,c,2',c,3',c,4',(,x,O,x,),x,c,5',c,6',Ring,Ring4
 mresolphthalein root root
 C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,
 Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(O),x,c,3',c,4',(,x,C,x,),x,c,5',c,6',
 Ring,Ring3,),x,c,1'',Ring,Ring4,c,2',(O),x,c,3',c,4',(,x,C,x,),x,c,5',c,6',Ring,Ring4
 cresolphthalein root root
 C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,
 Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(,x,C,x,),x,c,5',c,6',
 Ring,Ring3,),x,c,1'',Ring,Ring4,c,2',c,3',(O),x,c,4',(,x,C,x,),x,c,5',c,6',Ring,Ring4

pyrocatecholphthalein root root
 C,1,Ring, Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring
 2,Ring, Ring1,),x,(,x,c,1',Ring, Ring3,c,2',c,3',(O),x,c,4',(,x,O,x,),x,c,5',c,6',
 Ring, Ring3,),x,c,1'',Ring, Ring4,c,2'',c,3'',(O),x,c,4'',(,x,O,x,),x,c,5'',c,6'',
 Ring, Ring4
 pyrogallolphthalein root root
 C,1,Ring, Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring
 2,Ring, Ring1,),x,(,x,c,1',Ring, Ring3,c,2',(,x,O,x,),x,c,3',(O),x,c,4',(,x,O,x,),
 x,c,5',c,6',Ring, Ring3,),x,c,1'',Ring, Ring4,c,2'',(,x,O,x,),x,c,3'',(O),x,c,4'',
 (,x,O,x,),x,c,5'',c,6'',Ring, Ring4
 thymolphthalein root root
 C,1,Ring, Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring
 2,Ring, Ring1,),x,(,x,c,1',Ring, Ring3,c,2',(,x,C(C)C,x,),x,c,3',c,4',(,x,O,x,),x,
 c,5',(C),x,c,6',Ring, Ring3,),x,c,1'',Ring, Ring4,c,2'',(,x,C(C)C,x,),x,c,3'',c,4'
 ',(,x,O,x,),x,c,5'',(C),x,c,6'',Ring, Ring4
 tetraiodophthalein|iodophthalein|iodophene|iodotetragnost root root
 C,1,Ring, Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring, Ring2,c,4,(I),x,c,5,(I),x,c,6,(I),x,
 c,7,(I),x,c,7a,Ring, Ring2,Ring, Ring1,),x,(,x,c,1',Ring, Ring3,c,2',c,3',c,4',(,x,
 O,x,),x,c,5',c,6',Ring, Ring3,),x,c,1'',Ring, Ring4,c,2'',c,3'',c,4'',(,x,O,x,),x,
 c,5'',c,6'',Ring, Ring4
 fluorescein root root
 C,1,Ring, Ring1,Ring, Ring5,(,x,O,2,C,3,(=O),x,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7
 a,Ring, Ring2,Ring, Ring1,),x,c,10a,Ring, Ring3,c,1',c,2',c,3',(,x,O,x,),x,c,4',c,4
 a',Ring, Ring3,O,x,c,5b',Ring, Ring4,c,5',c,6',(,x,O,x,),x,c,7',c,8',c,8a',Ring, Ri
 ng5,Ring, Ring4
 sulfonfluorescein root root
 C,1,Ring, Ring1,Ring, Ring5,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7
 ,c,7a,Ring, Ring2,Ring, Ring1,),x,c,10a,Ring, Ring3,c,1',c,2',c,3',(,x,O,x,),x,c,4'
 ,c,4a',Ring, Ring3,O,x,c,5b',Ring, Ring4,c,5',c,6',(,x,O,x,),x,c,7',c,8',c,8a',Rin
 g, Ring5,Ring, Ring4
 fluoran|fluorane root root
 C,1,Ring, Ring1,Ring, Ring5,(,x,O,2,C,3,(=O),x,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7
 a,Ring, Ring2,Ring, Ring1,),x,c,10a,Ring, Ring3,c,1',c,2',c,3',c,4',c,4a',Ring, Ring
 3,O,x,c,5b',Ring, Ring4,c,5',c,6',c,7',c,8',c,8a',Ring, Ring5,Ring, Ring4
 uramil root root N,n,C1C(=O)NC(=O)NC(=O)1,x
 isosorbide root root
 O,x,[C@H],2,Ring, Ring1,C,1,O,x,[C@H],4,Ring, Ring2,(,x,[H],x,),x,[C@],3,Ring, Ring
 1,(,x,[H],x,),x,O,x,C,6,[C@H],5,Ring, Ring2,O,x
 isoproterenol|isoprenaline root root CC(NCC(C1=CC(O)=C(O)C=C1)O)C,x
 shikonin root root CC(C)=CC[C@H](O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
 alkannin root root CC(C)=CC[C@H](O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
 shikalkin root root CC(C)=CCC(O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
 hyoscyamine root root CN1C2CCC1C[C@H](OC(C(CO)c3cccc3)=O)C2,x
 44'carbocyanine|cryptocyanine|kryptocyanine root root
 [n+],1,Ring, Ring1,c,2,c,3,c,4,(,x,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring
 2,Ring, Ring1,),x,C=CC=,x,C,4',Ring, Ring3,C,3',=,x,C,2',N,1',c,8a',Ring, Ring4,c,8
 ',c,7',c,6',c,5',c,4a',Ring, Ring4,Ring, Ring3
 22'carbocyanine|pinacyanol root root
 [n+],1,Ring, Ring1,c,2,(,x,c,3,c,4,c,4a,Ring, Ring2,c,5,c,6,c,7,c,8,c,8a,Ring, Ring
 2,Ring, Ring1,),x,C=CC=,x,C,2',(,x,C,3',=,x,C,4',Ring, Ring3,),x,N,1',c,8a',Ring, R
 ing4,c,8',c,7',c,6',c,5',c,4a',Ring, Ring4,Ring, Ring3
 oxacarbocyanine root root
 o,1,Ring, Ring1,c,2,(,x,[n+],3,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring2,Ri
 ng, Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring, Ring3,N,3',c,3a',Ring, Ring4,c,4',c,5
 ',c,6',c,7',c,7a',Ring, Ring4,O,1',Ring, Ring3
 oxadicarbocyanine root root
 o,1,Ring, Ring1,c,2,(,x,[n+],3,c,3a,Ring, Ring2,c,4,c,5,c,6,c,7,c,7a,Ring, Ring2,Ri

ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
 Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
 oxatricarbocyanine root root
 o,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
 3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
 thiacyanine root root
 s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,),x,C,8,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c
 ,7a',Ring,Ring4,S,1',Ring,Ring3
 thiacarbocyanine root root
 s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5
 ',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
 thiadicarbocyanine root root
 s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
 Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
 thiatricarbocyanine root root
 s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
 3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
 selenacarbocyanine root root
 [se],1,Ring,Ring1,cc,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
 2,Ring,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4'
 ,c,5',c,6',c,7',c,7a',Ring,Ring4,[Se],1',Ring,Ring3
 hordenine root root CN(C)CCC1=CC=C(O)C=C1,x
 maltol root root O1CCC(=O)C(O)C(C)1,x
 coman root root Cc1=cc(=O)cc01,x
 chrysoidine root root
 c,4|p|para,(,x,c,3|m|meta,c,2|o|ortho,Ring,Ring1,),x,c,5,c,6,c,1,Ring,Ring1,N=Nc
 2c(N)cc(N)cc2,x
 alphafuril root root O=C(C1=CC=CO1)C(C2=CC=CO2)=O,x
 anisil root root O=C(C1=CC=C(OC)C=C1)C(C2=CC=C(OC)C=C2)=O,x
 alphaphellandrene root root CC1=CCC(C(C)C)C=C1,x
 betaphellandrene root root CC(C(C=C1)CCC1=C)C,x
 scopolamine|scopolamin root root C[N+]1([O-
])C2CCC1CC(OC(C(CO)C3=CC=CC=C3)=O)C2,x
 pilocarpine|pilocarpin root root CC[C@H]1[C@H](CC2=CN=CN2C)COCl=O,x
 guanethidine root root NC(NCCN1CCCCCCCC1)=N,x
 lobeline root root CN1C(CC(C3=CC=CC=C3)O)CCCC1CC(C2=CC=CC=C2)=O,x
 mercaptur root root C[C@H](CS)NC(C)=O,x
 phenylmercaptur root root C[C@H](CSc1cccc1)NC(C)=O,x
 alphilip|alip root root CCCCCC1SSCC1,x
 perill|perilla root root CC1=CCC(C(C)=C)CC1,x
 biotin root root O,1@x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
 biotinyl root root C,4@x,(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
 biotinamide|biotinamid root root
 N,x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
 bisphenola root root
 O1.Oc,4,Ring,Ring2,c,5,c,6,c,1,(,x,c,2,c,3,Ring,Ring2,),x,C(C)(C),x,c,1',Ring,Ri
 ng3,c,2',c,3',c,4',Ring,Ring1,c,5',c,6',Ring,Ring3
 pantothen root root CCCNC(C(C(CO)(C)C)O)=O,x
 allophan root root
 N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,(=O),x,C,5,(=O),x,C,6,(=O),x,Ring,Ring1
 croman root root Cc1occc(=O)c1,x

cinchon root root
 C,9,(,x,c,4',Ring,Ring2,c,4a',(,x,c,5',c,6',c,7',c,8',Ring,Ring4,),x,c,8a',Ring,
 Ring4,n,1'|a-1,c,2'|a-b,c,3'|a-
 t,Ring,Ring2,),x,C,8,Ring,Ring1,N(CC3)CC(,x,C,10,=,x,C,11,)C3C1,x
 1011dihydrocinchon root root
 C,9,(,x,c,4',Ring,Ring2,c,4a',(,x,c,5',c,6',c,7',c,8',Ring,Ring4,),x,c,8a',Ring,
 Ring4,n,1'|a-1,c,2'|a-b,c,3'|a-
 t,Ring,Ring2,),x,C,8,Ring,Ring1,N(CC3)CC(,x,C,10,C,11,)C3C1,x
 cinchonine|cinchonin root root
 O[C@H]([C@H]2N(CC4)C[C@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
 1011dihydrocinchonine|1011dihydrocinchonin root root
 O[C@H]([C@H]2N(CC4)C[C@H](CC)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
 quinidine root root
 O[C@H]([C@H]2N(CC4)C[C@H](C=C)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
 1011dihydroquinidine root root
 O[C@H]([C@H]2N(CC4)C[C@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
 cinchonidine|cinchonidin root root
 O[C@H]([C@H]2N(CC4)C[C@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
 1011dihydrocinchonidine|1011dihydrocinchonidin root root
 O[C@H]([C@H]2N(CC4)C[C@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
 quinine|quinin root root
 O[C@H]([C@H]2N(CC4)C[C@H](C=C)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
 1011dihydroquinine|1011dihydroquinin|dihydroquinine|dihydroquinin|hydroquinine|h
 ydroquinin root root
 O[C@H]([C@H]2N(CC4)C[C@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
 hepes root root S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o,),x,CCN(CC1)CCN1CCO,x
 pipes root root O=S(CCN1CCN(CCS(=O)(O)=O)CC1)(O)=O,x
 popop root root C1(C2=CC=C(C4=NC=C(C5=CC=CC=C5)O4)C=C2)=NC=C(C3=CC=CC=C3)O1,x
 dibenzosuber root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
 ,9a,Ring,Ring3,c,10,C,11,c,11a,Ring,Ring2,Ring,Ring1
 benzosuber root root
 C,1,Ring,Ring1,C,2,C,3,C,4,C,5,c,5a,Ring,Ring2,c,6,c,7,c,8,c,9,c,9a,Ring,Ring2,R
 ing,Ring1
 orthosilicate root root
 [Si],x,(,x,O,1@o''',),x,(,x,O,1@o'''),x,(,x,O,1@o'''),x,O,1@o
 orthotitanate root root
 [Ti],x,(,x,O,1@o''',),x,(,x,O,1@o'''),x,(,x,O,1@o'''),x,O,1@o
 gona|gon root steroid
 C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,c,6,C,7,C,8,Ring,Ring3,C,14,Ri
 ng,Ring4,C,15,C,16,C,17,C,13,Ring,Ring4,C,12,C,11,C,9,Ring,Ring3,C,10,Ring,Ring1
 ,Ring,Ring2
 estra|oestra|estr root steroid
 C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,c,6,C,7,C,8,Ring,Ring3,C,14,Ri
 ng,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C,9,Ring,Ring3
 ,C,10,Ring,Ring1,Ring,Ring2
 equilen root steroid
 c,3,(O)(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,c,6,c,7,c,8,Ring,Ring3,C,14
 ,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C,9,
 Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
 dihydroequilen root steroid
 c,3,(O)(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,c,6,c,7,c,8,Ring,Ring3,C,14
 ,Ring,Ring4,C,15,C,16,C,17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C,9,R
 ing,Ring3,c,10,Ring,Ring1,Ring,Ring2
 androsta|androst|etiochola|etiochol root steroid
 C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,c,6,C,7,C,8,Ring,Ring3,C,14,Ri

ng, Ring4, C, 15, C, 16, C, 17, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 etioallochola|etioallochol root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, [C@@], 5, ([H]), x, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, C, 17, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 etien root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, =, x, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (C), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 androstanedione root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@H], 17, (O), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 pregnane root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, =, x, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, C, 20, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 allopregnane root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, [C@@], 5, ([H]), x, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, C, 20, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 cholane root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@H], 20, (, x, C, 22, C, 23, C, 24,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 cholesta|cholest|coprost root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@], 20, (, x, C, 22, C, 23, C, 24, C, 25, (, x, C, 26,), x, C, 27,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 lanosta|lanost root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, [C@], 4, (, x, C, 28,), (, x, C, 29,), x, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, [C@], 14, Ring, Ring4, (, x, C, 30,), x, C, 15, C, 16, [C@], 17, (, x, [C@@], 20, (, x, C, 22, C, 23, C, 24, C, 25, (, x, C, 26,), x, C, 27,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 dammarane root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, [C@], 4, (, x, C, 28,), (, x, C, 29,), x, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, [C@@], 14, Ring, Ring4, (, x, C, 30,), x, C, 15, C, 16, [C@], 17, (, x, [C@@], 20, (, x, C, 22, C, 23, C, 24, C, 25, (, x, C, 26,), x, C, 27,), x, C, 21,), x, [C@@], 13, Ring, Ring4, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
 ursane root steroid
 C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, (, x, C, x,), (, x, C, x,), x, C, 5, Ring, Ring2, C, 6, C, 7, [C@], 8, (C), x, Ring, Ring3, [C@], 14, Ring, Ring4, (C), 27, C, x, C, x, [C@@], x, Ring, Ring5, (C), 28, C, 22, C, 21, [C@H], 20, (, x, C, 30,), x, [C@H], 19, (, x, C, 29,), x, [C@@], 18, ([H]), x, Ring, Ring5, [C@@], 13, Ring, Ring4, (, x, [H], x,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, x

lup root steroid
C,3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,(.x,C,x,)(.x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(C),27,C,x,C,x,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,[C@H],19,(.x,C,20,(.x,C,29,),x,C,30,),x,[C@@],18,([H]),x,Ring,Ring5,[C@],13,Ring,Ring4,(.x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,x
 taraxaster root steroid
C,3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,(.x,C,x,)(.x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(.x,C,x,),x,C,x,C,x,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,C,20,(=x,C,30,),x,C,19,(.x,C,29,),x,[C@],18,([H]),x,Ring,Ring5,[C@],13,Ring,Ring4,(.x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,x
 oleane|olean root steroid
C,3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,(.x,C,23,)(.x,C,24,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(.x,C,x,),x,C,15,C,16,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,C,20,(.x,C,30,)(.x,C,29,),x,C,x,[C@@],18,([H]),x,Ring,Ring5,[C@],13,Ring,Ring4,(.x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 olean loveracid steroid
C,x,Ring,Ring6,..,x,C,3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,(.x,C,23,)(.x,C,24,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(.x,C,x,),x,C,15,C,16,[C@@],x,Ring,Ring5,Ring,Ring6,C,x,C,x,C,x,(.x,C,x,)(.x,C,29,),x,C,x,[C@],x,([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,=,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 olean|oleanol loveracid steroid
C,x,Ring,Ring6,..,x,[C@H],3,(O)(.x,C,2,C,1,Ring,Ring1,),x,C,4,(.x,C,23,)(.x,C,24,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(.x,C,x,),x,C,15,C,16,[C@@],x,Ring,Ring5,Ring,Ring6,C,x,C,x,C,x,(.x,C,x,)(.x,C,29,),x,C,x,[C@],x,([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,=,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 glycyrrhetin root steroid
C,29,Ring,Ring6,..,x,[C@],3,(O),x,(.x,C,2,C,1,Ring,Ring1,),x,C,4,(.x,C,x,)(.x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(.x,C,x,),x,C,x,C,x,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,[C@],20,(.x,C,30,),x,Ring,Ring6,C,x,[C@@],18,([H]),x,Ring,Ring5,C,13,Ring,Ring4,=,x,C,12,C,11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 glycyrrhet root steroid
C,29,Ring,Ring6,..,x,[C@],3,(O),x,(.x,C,2,C,1,Ring,Ring1,),x,C,4,(.x,C,x,)(.x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(.x,C,x,),x,C,x,C,x,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,[C@],20,(.x,C,30,),x,Ring,Ring6,C,x,[C@@],18,([H]),x,Ring,Ring5,C,13,Ring,Ring4,=,x,C,12,C,11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 solanid root steroid
C,3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,[C@],8,([H]),x,Ring,Ring3,[C@@],14,([H]),x,Ring,Ring4,C,15,[C@@],16,([H]),x,Ring,Ring5,N,28,Ring,Ring6,C,x,[C@@],25,(C),x,C,24,C,23,[C@@],22,([H]),x,Ring,Ring6,[C@@],x,(C),x,[C@@],x,([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,(C),18,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,x
 cholester root steroid
C,3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,c,5,Ring,Ring2,c,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(.x,[C@@H],20,(.x,C,22,C,23,C,24,C,25,(.x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(.x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 lanoster root steroid
C,3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,(.x,C,28,)(.x,C,29,),x,C,5,Ring,Ring2,=,x,C,6,C,7,C,8,Ring,Ring3,[C@],14,Ring,Ring4,(.x,C,30,),x,C,15,C,16,[C@],17,(.x,[C@@H]

,20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 ergosta|ergost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Rin g3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 campesta|campest root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ri ng3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 poriferasta|poriferast root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(CC),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ri ng3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 stigmasta|stigmast root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(,x,C,28,C,29,),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 pregnenolone root steroid
C,1,Ring,Ring1,C,2,C,3,(O),x,C,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin g,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 prednisolone|prednisolon root steroid
C,1,Ring,Ring1,=,x,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,(,x,O,x,),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 progestrone|progesteron root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin g,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 tetrahydroprogesterone|tetrahydroprogesteron root steroid
C,1,Ring,Ring1,C,2,C,3,(O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin g,Ring4,C,15,C,16,[C@],17,(,x,C,20,(O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 hydrocortisone|hydrocortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin g,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Rin g,Ring4,(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Rin g,Ring2,C,19
 dihydrocortisone|dihydrocortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin g,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Rin g,Ring4,(,x,C,18,),x,C,12,[C@H],11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Rin g,Ring2,C,19
 tetrahydrocortisone|tetrahydrocortison root steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin g,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Rin g,Ring4,(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Rin g,Ring2,C,19
 cortisone|cortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin g,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13

,Ring,Ring4,(,x,C,18,),x,C,12,[C@H],11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring
 1,Ring,Ring2,C,19
 androsterone root steroid
 C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
 ,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9
 ,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 isoandrosterone root steroid
 C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
 ,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9
 Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 aldosterone root steroid
 C,3,(,x,C,2,C,1,Ring,Ring1,) (=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
 4,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,1
 8,=O,x,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,1
 9
 pregnanolone root steroid
 C,3,(O)(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
 ,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,
 18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 testosteron|testosterone root steroid
 C,3,(,x,C,2,C,1,Ring,Ring1,) (=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
 4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
 C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 dihydrotestosteron|dihydrotestosterone root steroid
 C,3,(,x,C,2,C,1,Ring,Ring1,) (=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
 4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
 C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 oestradiol|estradiol|betaoestradiol|betaestradiol root steroid
 c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
 ,14,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11
 ,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
 oestriol|estriol root steroid
 c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
 ,14,Ring,Ring4,C,15,[C@@],16,(O),x,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x
 ,C,12,C,11,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
 oestrone|estrone root steroid
 c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
 ,14,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C
 ,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
 brassinolid|brassinolide root steroid
 [C@H],3,(O),x,(,x,[C@H],2,(O),x,C,1,Ring,Ring1,),x,C,4,[C@],5,Ring,Ring2,([H]),
 x,C,6,(=O)O,x,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,
 (,x,[C@H],22,(O),x,[C@H],23,(O),x,[C@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,2
 1,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
 ng1,Ring,Ring2,C,19
 calcidiol root root
 [C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
 Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C,2
 5,(,x,C,26,) (O),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
 ,9,Ring,Ring3,,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
 calcidiol|cholecalciferol|vitamind3 root root
 [C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8|
 a-
 r,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C
 ,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11|a-
 t,C,9|a-b,Ring,Ring3,,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19

calcitriol root root
[C@H]3,[O],x,(,x,C,2,[C@H],1,(O),x,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,)O),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
 corticosterone root steroid
C,3,(=O)(,x,C,2,C,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 cortisol root steroid
C,3,(=O)(,x,C,2,C,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 ecdysone root steroid
[C@H]3,(O),x,(,x,[C@H],2,(O),x,C,1,Ring,Ring1,),x,C,4,[C@@],5,Ring,Ring2,([H]),x,C,6,(=O),x,C,7,=,x,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
 ergocaliol|ergocaliferol root root
[C@H]3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,=,x,C,23,[C@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
 ergosterol root steroid
[C@H]3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,=,x,C,23,[C@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 lumisterol root steroid
[C@H]3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,=,x,C,23,[C@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,[C@],9,([H]),x,Ring,Ring3,[C@],10,Ring,Ring1,Ring,Ring2,C,19
 cardanolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,Ring,Ring5,C,21,O,x,C,23,(=O),x,C,22,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 card2022enolide|2022cardenolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,Ring,Ring5,C,21,O,x,C,23,(=O),x,C,22,=,x,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 digitoxigenin root steroid
O,x,[C@@],3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@],5,Ring,Ring2,([H]),x,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,Ring,Ring5,C,21,O,x,C,23,(=O),x,C,22,=,x,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 bufanolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,Ring,Ring5,C,21,O,x,C,24,(=O),x,C,23,C,22,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19

bufadienolide root steroid
C3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,C,16,[C@],17,(.x,[C@@],20,Ring,Ring5,=,x,C,21,O,x,C,24,(=O),x,C,23 ,=,x,C,22,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Rin g3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 cev root steroid
C3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,[C@@],1 4,([H]),x,Ring,Ring4,C,15,C,16,[C@@],17,([H]),x,Ring,Ring5,[C@H],20,(C),x,[C@@] ,x,([H]),x,Ring,Ring6,C,x,C,x,[C@H],x,(C),x,C,x,N,x,Ring,Ring6,C,x,[C@],x,([H]) ,x,Ring,Ring5,[C@@],12,([H]),x,Ring,Ring4,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1 ,Ring,Ring2,C,19
 solidan root steroid
C3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,C,16,Ring,Ring5,[C@],17,([H])(.x,[C@],20,(,x,C,21,),x,[C@],22,([H]),x,Ring,Ring6,C,23,C,24,[C@H],25,(,x,C,27,),x,C,26,N,28,Ring,Ring6,Ring,Ring5,) ,x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1 ,Ring,Ring2,C,19
 spirost root steroid
C3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,[C@],16,([H])(.x,O,x,Ring,Ring5,),x,[C@],17,([H])(.x,[C@@],20,(,x, [C@@],22,Ring,Ring5,(.x,O,x,Ring,Ring6,),x,C,23,C,24,C,25,(,x,C,26,Ring,Ring6,),x ,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C @@],10,Ring,Ring1,Ring,Ring2,C,19
 spirosol root steroid
C3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,[C@],16,([H])(.x,O,x,Ring,Ring5,),x,[C@],17,([H])(.x,[C@@],20,(,x, [C@@],22,Ring,Ring5,(.x,N,x,Ring,Ring6,),x,C,23,C,24,C,25,(,x,C,26,Ring,Ring6,),x ,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C @@],10,Ring,Ring1,Ring,Ring2,C,19
 tomatid root steroid
C3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,[C@H],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring ,Ring3,C,14,Ring,Ring4,C,15,[C@],16,([H])(.x,O,x,Ring,Ring5,),x,[C@],17,([H])(.x, [C@],20,(,x,[C@@],22,Ring,Ring5,(.x,N,x,Ring,Ring6,),x,C,23,C,24,[C@H],25,(,x,C ,26,Ring,Ring6,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C ,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 solasod root steroid
C3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,[C@H],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring ,Ring3,C,14,Ring,Ring4,C,15,[C@],16,([H])(.x,O,x,Ring,Ring5,),x,[C@],17,([H])(.x, [C@],20,(,x,[C@@],22,Ring,Ring5,(.x,N,x,Ring,Ring6,),x,C,23,C,24,[C@H],25,(,x,C ,26,Ring,Ring6,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C ,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 furost root steroid
C3,(.x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri ng,Ring4,C,15,[C@],16,([H])(.x,O,x,Ring,Ring5,),x,[C@],17,([H])(.x,[C@@],20,(,x, [C@@],22,Ring,Ring5,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,R ing4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 chol loveracid steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@H],7,(O),x,C,8,Ring ,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(.x,[C@H],20,(,x,C,22,C,23,C,24,),x,C,2 1,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,[C@H],12,(O),x,C,11,C,9,Ring,Ring3,[C@@] ,10,Ring,Ring1,Ring,Ring2,C,19
 lithochol loveracid steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14 ,Ring,Ring4,C,15,C,16,[C@],17,(.x,[C@H],20,(,x,C,22,C,23,C,24,),x,C,21,),x,[C@@] ,13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19

dehydrochol loveracid steroid
 C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,(=O),x,C,8,Ring,Ring3,C
 ,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21,),x,[
 C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,(=O),x,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
 ng1,Ring,Ring2,C,19
 hyodeoxychol loveracid steroid
 C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,[C@@H],6,(O),x,C,7,C,8,Ring
 ,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,
 21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
 ng1,Ring,Ring2,C,19
 chenodeoxychol loveracid steroid
 C,1,Ring,Ring1,C,2,C,3,[C@@H],4,(O),x,C,5,Ring,Ring2,C,6,[C@@H],7,(O),x,C,8,Ring
 ,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,
 21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
 ng1,Ring,Ring2,C,19
 ursodeoxychol loveracid steroid
 C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@H],7,(O),x,C,8,Ring,Ri
 ng3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21
 ,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Rin
 g1,Ring,Ring2,C,19
 tauroursodeoxychol loveracid steroid
 S,x,(=O),x,(=O),x,(,x,O,1@x,),x,C,x,C,x,N,x,Ring,Ring5,..,x,C,1,Ring,Ring1,C,2,[C
 @@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@H],7,(O),x,C,8,Ring,Ring3,C,14,Ring,Ring4
 ,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=O),x,Ring,Ring5,),x,C,21,)
 ,x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
 Ring,Ring2,C,19
 taurochol loveracid steroid
 S,x,(=O),x,(=O),x,(,x,O,1@x,),x,C,x,C,x,N,x,Ring,Ring5,..,x,C,1,Ring,Ring1,C,2,C
 3,[C@H],4,(O),x,C,5,Ring,Ring2,C,6,[C@@H],7,(O),x,C,8,Ring,Ring3,C,14,Ring,Ring4
 ,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=O),x,Ring,Ring5,),x,C,21,)
 ,x,[C@@],13,Ring,Ring4,(,x,C,x,),x,[C@@H],12,(O),x,C,11,C,9,Ring,Ring3,[C@@],10,
 Ring,Ring1,Ring,Ring2,C,19
 glycochol loveracid steroid
 C,1,Ring,Ring1,C,2,C,3,[C@H],4,(O),x,C,5,Ring,Ring2,[C@@H],6,(O),x,C,7,C,8,Ring
 Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=O)NCC
 ,x,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,[C@@H],12,(O),x,C,11,C,9,Ring,Ri
 ng3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 oxymetholone root steroid
 C,3,(=O)(,x,C,2,(=CO),x,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ri
 ng3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(O)(C),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,
 C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
 homo natderiver nathomo x,x
 nor natderiver natnor x,x
 seco natderiver natseco x,x
 abeo natderiver natabeo x,x
 cyclo natderiver cyclo x,x
 rightarrow|arrow|fwdarrow|fwdarw unknown natarrow x,x
 flophemesyl root root [Si],4@x,(C)(C)c1c(F)c(F)c(F)c(F)c(F)1,x
 diethylenetriamine root root N,n|1,C,2,C,3,N,n''|4,C,5,C,6,N,n'|7
 triethylenetetramine root root N,n,CC,x,N,n'',CC,x,N,n''',CC,x,N,n'''',CC,x,N,n'
 tetraethylennepentamine root root
 N,n,CC,x,N,n''',CC,x,N,n''',CC,x,N,n'''',CC,x,N,n'''''',CC,x,N,n'
 pentaethylenehexamine root root
 N,n,CC,x,N,n''',CC,x,N,n''',CC,x,N,n'''',CC,x,N,n''''',CC,x,N,n'
 cupferron root root O=NN([O-])c1ccccc1.[NH4+],x
 camphene root root C=C(CC(CC2)C1(C)C)C12C,x

isopinocamphe root root
 C,3,Ring,Ring1,C,4,C,5,(.x,C,6,Ring,Ring2,),x,C,7,(C)(C),x,C,1,Ring,Ring2,C,2,(C),x,Ring,Ring1
 choline root root O,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
 phosphocholine root root O,1@x,P,x,(=O),x,([O-]),x,O,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
 diphosphocholine root root O,1@x,P,x,(=O),x,(.x,O,1@x,),x,O,x,P,x,(=O),x,([O-]),x,O,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
 phosphoethanolamine root root O,1@x,P,x,(=O),x,(O),x,O,x,C,b|beta,C,a|alpha,N,x
 fluorocholine root root F,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
 chlorocholine root root Cl,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
 bromocholine root root Br,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
 iodocholine root root I,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
 betaine|betain root root [O-],x,C,x,(=O),x,C,a|alpha,[N+](C)(C)C,x
 betainealdehyde|betainaldehyd root root [H],x,C,x,(=O),x,C,a|alpha,[N+](C)(C)C,x
 carnitine|carnitin root root O,1@o,Ring,Ring1,.,x,[O-],x,C,x,(=O),x,C,a|alpha,C,b|beta,Ring,Ring1,C,g|gamma,[N+](C)(C)C,x
 carnitinamide root root
 N,x,C,x,(=O),x,C,a|alpha,C,b|beta,(O),1@o,C,g|gamma,[N+](C)(C)C,x
 aminocarnitine|aminocarnitin root root [O-],x,C,x,(=O),x,C,a|alpha,C,b|beta,(N),x,C,g|gamma,[N+](C)(C)C,x
 exact-azine root root n1cccc1,x
 exact-ether root root CCOCC,x
 exact-alcohol root root OCC,x
 exact-salt root root [Na+].[Cl-],x
 exact-sulfur root root S1SSSSSS1,x
 exact-phenazo root root OC(C=C4)=CC=C4N=NC(C([N+]([O-])=O)=C=C2C1=CC([N+]([O-])=O)=C(N=NC3=CC=C(O)C=C3)C=C1,x
 exact-nitron root root C2([N-]N(C4=CC=CC=C4)C=[N+]2C3=CC=CC=C3)=NC1=CC=CC=C1,x
 exact-anthranyl root root c1onc2ccccc12,x
 exact-acetal root root CC(OCC)OCC,x
 exact-sugar root root
 OC[C@H]1([C@H](O)[C@H](O)[C@H](O1)CO)O[C@H]2[C@H](O)[C@H](O)[C@H](O)[C@H](CO)O2,x
 exact-bisacrylamide root root O=C(C=C)NCNC(C=C)=O,x
 exact-dopa root root
 C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,c,x,Ring,Ring2,c,
 2|o|ortho,c,3|m|meta,(O),x,c,4|p|para,(O),x,c,5,c,6,Ring,Ring2
 exact-hydrogen root root [H][H],x
 exact-deuterium root root [2H][2H],x

 zircon root root
 O[S](=O)(C1=CC(N=NC(C3=CC=CC=C3)=NNC2=CC=CC=C2C(O)=O)=C(O)C=C1)=O,x
 chloroform root chloroform C([H])(Cl)(Cl)Cl,x
 fluoroform root chloroform C([H])(F)(F)F,x
 bromoform root chloroform C([H])(Br)(Br)Br,x
 iodoform root chloroform C([H])(I)(I)I,x
 ferricyanide root root [Fe-3](C#N)(C#N)(C#N)(C#N)(C#N)(C#N),x
 ferrocyanide root root [Fe-4](C#N)(C#N)(C#N)(C#N)(C#N)(C#N)(C#N),x
 dibromochloride root root [Cl-](Br)Br,x
 dibromoiodide root root [I-](Br)Br,x
 dichloroiodate|dichloroiodide root root [I-](Cl)Cl,x
 diiodoaurate root root [Au-](I)I,x
 dichloroaurate root root [Au-](Cl)Cl,x
 dibromoaurate root root [Au-](Br)Br,x
 bromodiiodide root root [Br-](I)I,x
 dichlorobromide root root [Br-](Cl)Cl,x

tetrachloroiodate|iodotetrachloride root root [I-](Cl)(Cl)(Cl)Cl,x
 chlorochromate root root [O-][Cr](=O)(=O)Cl,x
 fluorochromate root root [O-][Cr](=O)(=O)F,x
 fluoroborate|fluorborat|tetrafluoroborate|tetrafluoroborate1|tetrafluoroborat|b
 f4|borofluoride|borofluorid|fluoborate|fluoborat root root [B-](F)(F)(F)F,x
 fluorosilicate|fluorosilicat|hexafluorosilicate|hexafluorosilicat root root [Si-]
 -(F)(F)(F)F,x
 borohydride|borohydrid root root [B-],x
 borodeuteride|borodeuterid root root [B-]([2H])([2H])([2H])[2H],x
 cyanoborodeuteride|cyanoborodeuterid root root [B-]([2H])([2H])([2H])C#N,x
 aluminohydride|aluminohydrid root root [Al-],x
 persulfate|persulfat|peroxodisulfate|peroxodisulfat root root
 O,1@x,S(=O)(=O)OOS(=O)(=O),x,O,1@x
 bifluoride|bifluorid root root [F-],x,.[H]F,x
 water root root [H]O[H],x
 hydrofluoride root hydrochloride [H]F,x
 hydrochloride|hcl root hydrochloride [H]Cl,x
 2hcl root hydrochloride [H]Cl.[H]Cl,x
 3hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl,x
 4hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl.[H]Cl,x
 5hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl.[H]Cl.[H]Cl,x
 methochloride|chlormethylate root hydrochloride CCl,x
 methobromide|brommethylate root hydrochloride CBr,x
 hydrobromide|hbr root hydrochloride [H]Br,x
 2hbr root hydrochloride [H]Br.[H]Br,x
 3hbr root hydrochloride [H]Br.[H]Br.[H]Br,x
 4hbr root hydrochloride [H]Br.[H]Br.[H]Br.[H]Br,x
 5hbr root hydrochloride [H]Br.[H]Br.[H]Br.[H]Br.[H]Br,x
 hydrotribromide|hbr root hydrochloride [H]Br(Br)Br,x
 hydroiodide|hydriodide root hydrochloride [H]I,x
 methiodide|methiodide root hydrochloride CI,x
 ethiodide|ethiodide root hydrochloride CCI,x
 hydrate|h2o root hydrochloride [H]O[H],x
 deuterate|d2o root hydrochloride [2H]O[2H],x
 etherate root hydrochloride
 O(C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H],x
 bitartarate|bitartrate|hydrogentartrate root hydrochloride
 O,1@x,C,1,(=,x,O,x,),x,C,2,(,x,O,x,),x,C,3,(,x,O,x,),x,C,4,(=,x,O),x,O,x,[H],x
 dbitartrate|hydrogendtartrate root hydrochloride
 O,1@x,C,1,(=,x,O,x,),x,[C@H],2,(,x,O,x,),x,[C@H],3,(,x,O,x,),x,C,4,(=,x,O),x,O,
 x,[H],x
 lbitartrate|hydrogenltartrate root hydrochloride
 O,1@x,C,1,(=,x,O,x,),x,[C@H],2,(,x,O,x,),x,[C@H],3,(,x,O,x,),x,C,4,(=,x,O),x,O,
 x,[H],x
 bimaleate|hydrogenmaleate root hydrochloride
 O,1@x,C,1,(=,x,O,x,),x,C,2,=,x,C,3,\,x,C,4,(=,x,O),x,O,x,[H],x
 bisuccinate|hydrogensuccinate root hydrochloride
 O,1@x,C,1,(=,x,O,x,),x,C,2,C,3,C,4,(=O)O[H],x
 bipthalate root hydrochloride
 O,1@x,C(=O),x,c,1,Ring,Ring1,c,2,(C(=O)O[H]),x,c,3,c,4,c,5,c,6,Ring,Ring1
 hydrogenoxalate root hydrochloride
 O,1@x,C,1,(=,x,O,x,),x,C,2,(=,x,O),x,O,x,[H],x
 bisulfate|bisulfat|hydrogensulfate root root O,1@x,S(=O)(=O)O[H],x
 bisulfite|bisulfit|hydrogensulfite root root O,1@x,S(=O)O[H],x
 bisulfide|bisulfid|hydrogensulfide root root S,1@x,[H],x
 glycol|cellosolve|cellosolv root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,O,1@x,,x,O,1@x,Ring,Ring1

thioglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,S,1@x,.,x,O,1@x,Ring,Ring1
 dithioglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2 b|beta,S,1@x,.,x,S,1@x,Ring,Ring1
 selenoglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Se],1@x,.,x,O,1@x,Ring,Ring1
 diselenoglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Se],1@x,.,x,[Se],1@x,Ring,Ring1
 telluroglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Te],1@x,.,x,O,1@x,Ring,Ring1
 ditelluroglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Te],1@x,.,x,[Te],1@x,Ring,Ring1
 tempo root root
 C,4,Ring,Ring1,C,5,C,6,(C)(C),x,N,1,(,x,O,16@x,),x,C,2,(C)(C),x,C,3,Ring,Ring1
 proxyl root root
 C,3,Ring,Ring1,C,2,(C)(C),x,N,1,(,x,O,16@x,),x,C,5,(C)(C),x,C,4,Ring,Ring1
 nitroxide|nitroxyl root root N,n,O,16@x
 nitramine root root N,n,[N+] (=O) [O-],x
 nitramino root root N,4@n,[N+] (=O) [O-],x
 special-oxine root root
 n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,(O),x,c,8a,Rin
 g,Ring1,Ring,Ring2
 special-azine|ketazine root azine N,8@x,N,8@x
 oxime|oxim|antioxime root oxime N,8@x,O,o
 hydrazone|hydrazon root oxime N,8@x,N,n
 semicarbazone|semicarbazon root oxime N,8@1,N,2,C,3,(=,x,O,x,),x,N,4
 azino root bridge N,8@x,N,8@x
 azimino root bridge N,4@x,N,x,=,x,N,4@x
 biimino|biimin root bridge N,4@x,N,4@x
 epidioxy root bridge O,4@x,O,4@x
 epidithio|epidithi root bridge S,4@x,S,4@x
 epimino root bridge N,5@x
 epithio root bridge S,5@x
 episeleno root bridge [Se],5@x
 epitelluro root bridge [Te],5@x
 epithioximino|epithioximin root bridge S,4@x,O,x,N,4@x
 epoxy root bridge O,5@x
 epoxyimino|epoxyimin root bridge O,4@x,N,4@x
 epoxynitrilo root bridge O,4@x,N,8@x
 epoxythio|epoxythi root bridge O,4@x,S,x,O,4@x
 epoxythioxy root bridge O,4@x,S,x,O,4@x
 epitrithio|epitrithi root bridge S,4@x,S,x,S,4@x
 cyanohydrin root oxime O,4@x,.,x,C,4@x,#N,x
 fluorohydrin root oxime O,4@x,.,x,F,4@x
 chlorohydrin root oxime O,4@x,.,x,Cl,4@x
 bromohydrin root oxime O,4@x,.,x,Br,4@x
 iodohydrin root oxime O,4@x,.,x,I,4@x
 acetal|ketal|semiacetal|demiacetal|hemicetal|semiketal|demiketal|hemiketal|glyc
 olacetal|glycolketal root oxime O,4@x,.,x,O,4@x
 mercaptal|mercaptole root oxime S,4@x,.,x,S,4@x
 ketone|keton root ketone C,x,=,x,O,x
 ketoxime root ketone C,x,=,x,N,x,O,x
 ketoximino root ketone C,x,=,x,N,x,O,4@x
 ketyl root ketone C,4@x,[O-],x
 sulfoxide|sulfoxid root ketone S,x,=,x,O,x
 sulfone|sulfon root ketone S,x,(=,x,O,x,),x,=,x,O,x
 sulfimide|sulfimid|sulfilimine|sulfilimin root ketone S,x,=,x,N,x

sulfoximide|sulfoximid|sulfoximine|sulfoximin root ketone
S,x,(=,x,O,x,),x,=,x,N,x
selenoxide|selenoxid root ketone [Se],x,=,x,O,x
selenone|selenon root ketone [Se],x,(=,x,O,x,),x,=,x,O,x
selenimide|selenimid root ketone [Se],x,=,x,N,x
selenoximide|selenoximid root ketone [Se],x,(=,x,O,x,),x,=,x,N,x
telluroxide|telluroxid root ketone [Te],x,=,x,O,x
tellurone|telluron root ketone [Te],x,(=,x,O,x,),x,=,x,O,x
tellurimide|tellurimid root ketone [Te],x,=,x,N,x
telluroximide|telluroximid root ketone [Te],x,(=,x,O,x,),x,=,x,N,x
peroxide|peroxid root ketone O,x,O,x
persulfide|persulfid root ketone S,x,S,x
formal root ketone O,x,Ring,Ring1.,x,O,x,C,x,Ring,Ring1
ether root ether O,x
etherof root ofether O,x
thioether root ether S,x
selenoether root ether [Se],x
telluroether root ether [Te],x
oin oin unknown C,1@b|beta,(O),x,C,1@a|alpha,=O,x
ano methanomaker unknown x,x
quinone|quinon suffix quinone O,8@x
quinodimethane|quinodimethan suffix quinone C,10@x
radical radical unknown x,x
yl suffix yl 1,y1
ylidene|yliden|ilidene|iliden| suffix yl 2,y1
ylidyne|ylidyn|ilidyne|ilidyn suffix yl 3,y1
ane|an suffix ignore x,x
ine|in suffix ignore x,x
ene|en suffix bondchange 2,bond
yne|yn suffix bondchange 3,bond
thiol|ylthiol suffix suffix S,4@s
ol suffix olsuffix O,4@x
olate suffix suffix [O-],4@x
anethiolate|thiolato suffix suffix [S-],4@x
one|on suffix reqcarbon O,8@x
thione suffix reqcarbon S,8@x
selenone|selone suffix reqcarbon [Se],8@x
tellurone suffix reqcarbon [Te],8@x
imine root oxime N,8@n
imine imine suffix N,8@n
iminium root oxime [N+],8@x
iminium imine suffix [N+],8@x
glycol glycol unknown O,4@o,,,x,O,4@o'
thioglycol glycol unknown S,4@s,,,x,O,4@o
dithioglycol glycol unknown S,4@s,,,x,S,4@s'
selenoglycol glycol unknown [Se],4@x,,,x,O,4@x
diselenoglycol glycol unknown [Se],4@x,,,x,[Se],4@x
telluroglycol glycol unknown [Te],4@x,,,x,O,4@x
ditelluroglycol glycol unknown [Te],4@x,,,x,[Te],4@x
cyanohydrin glycol unknown C,4@x,#N,x,,,x,O,4@x
fluorohydrin glycol unknown F,4@x,,,x,O,4@x
chlorohydrin glycol unknown Cl,4@x,,,x,O,4@x
bromohydrin glycol unknown Br,4@x,,,x,O,4@x
iodohydrin glycol unknown I,4@x,,,x,O,4@x
oxide counterion oxide O,8@x
sulfide|mercaptide counterion oxide S,8@x
selenide counterion oxide [Se],8@x

telluride counterion oxide [Te], 8@x
 methanoxymethano root methanobridge C, 4@x, O, x, C, 4@x
 etheno root methanobridge C, 4@x, =, x, C, 4@x
 metheno root metheno C, 5@x
 obzeno root methanobridge c, 4@x, Ring, Ring1, c, 4@x, c, x, c, x, c, x, c, x, Ring, Ring1
 epoxide|enoxide counterion bridge O, 5@x
 episulfide counterion bridge S, 5@x
 sultam counterion bridge S, 4@x, (=, x, O, x,), x, (=, x, O, x,), x, N, 4@x
 sultone|sultone counterion bridge S, 4@x, (=, x, O, x,), x, (=, x, O, x,), x, O, 4@x
 dicarboximide|dicarboxylicimide|dicarboxylicacidimide counterion bridge
 C, 4@x, (=, x, O, x,), x, N, x, C, 4@x, =, x, O, x
 dicarboximido counterion bridge
 C, 4@x, (=, x, O, x,), x, Ring, Ring1, ., x, C, 4@x, Ring, Ring2, =, x, O, x, ., x, N, 4@x, Ring, Ring1,
 Ring, Ring2
 carbolactam counterion bridge C, 4@x, (=, x, O, x,), x, O, 4@x
 nitride counterion ionable N, 12@x
 phosphide counterion ionable P, 12@x
 antimonide counterion ionable [Sb], 12@x
 arsenide counterion ionable [As], 12@x
 hydroxide|hydroxid counterion ionable O, 4@x
 deuterioxide|deuteroxid counterion ionable O, 4@x, [2H], x
 hydrosulfide|hydrosulfid|sulphydrate|sulhydrat counterion ionable S, 4@x
 hydroselenide|hydroselenid counterion ionable [Se], 4@x
 hydrotelluride|hydrotellurid counterion ionable [Te], 4@x
 hydride|hydrid counterion ionable [H], 4@1
 deuteride|deuterid counterion ionable [2H], 4@1
 fluoride|fluorid counterion ionable F, 4@1
 chloride|chlorid|muriate counterion ionable Cl, 4@1
 bromide|bromid counterion ionable Br, 4@1
 iodide|iodid counterion ionable [I], 4@1
 acetylde counterion ionable C, 4@x, #[C-], x
 cyanide|cyanid counterion ionable C, 4@x, #N, x
 isocyanide|isocyanid|isonitrile counterion ionable [N+], 4@x, #[C-], x
 cyanate|cyanat counterion ionable O, 4@x, C#N, x
 isocyanate|isocyanat counterion ionable N, 4@x, =C=O, x
 fulminate|fulminat counterion ionable O, 4@x, [N+]#[C-], x
 thiocyanate|thiocyanat|sulfocyanate|sulfocyanat|sulfocyanide|sulfocyanid|rhodani
 de|rhodanid counterion ionable S, 4@x, C#N, x
 isothiocyanate|isothiocyanat|isorhodanide|isorhodanid counterion ionable
 N, 4@x, =C=S, x
 selenocyanate|selenocyanat counterion ionable [Se], 4@x, C#N, x
 isoselenocyanate|isoselenocyanat counterion ionable N, 4@x, =C=[Se], x
 tellurocyanate|tellurocyanat counterion ionable [Te], 4@x, C#N, x
 isotellurocyanate|isotellurocyanat counterion ionable N, 4@x, =C=[Te], x
 azide|azid counterion ionable N, 4@x, =[N+]=[N-], x
 sulfenamide|sulfenamid counterion counterion S, 4@x, N, n
 sulfonazide counterion counterion S, 4@x, (=O)(=O)N[N+][N-], x
 alcohol|icalcohol counterion counterion O, 4@x
 deuterol counterion counterion O, 4@x, [2H], x
 selenol counterion counterion [Se], 4@s
 tellurol counterion counterion [Te], 4@s
 nitrile|nitril counterion counterion N, 12@x
 carbonitrile|carbonitril counterion counterion C#N, 4@x
 diazonium counterion counterion [N+], 4@x, #N, x
 mercaptan|thioalcohol counterion counterion S, 4@x
 hydroperoxide|hydroperoxid counterion ionable O, 4@x, O, x

carboxaldehyde|carboxaldehyd|carboxyaldehyde|carboxyaldehyd|carbonal counterion
counterion C,4@x,(=O),x
carboxaldoxime|carboxaldoxim counterion counterion C,4@x,(=NO),x
carbamidine counterion counterion C,4@x,(=,x,N,1@n'|n2,),x,N,2@n|n1
oxyfluoride counterion bridge F,4@x,.,x,O,8@x
oxychloride counterion bridge Cl,4@x,.,x,O,8@x
oxybromide counterion bridge Br,4@x,.,x,O,8@x
oxyiodide counterion bridge I,4@x,.,x,O,8@x
thiocloride counterion bridge Cl,4@x,.,x,S,8@x
oxylradical counterion counterion O,20@x
carbo|carb carbeth root C,4@x,(=O),x
dioxyl infix infix O,4@x,O,x
oxy infix doublebondable O,4@x
peroxy infix doublebondable O,4@x,O,x
sulfanyl infix infix S,4@x
thio infix doublebondable S,4@x
mercapto infix infix S,4@x
seleno infix doublebondable [Se],4@x
telluro infix doublebondable [Te],4@x
amino|amin infix infix N,4@n|w|omega
phosphino infix infix P,4@n|w|omega
phosphinyl infix infix [PH3],4@x,(=,x,O,x,),x
arsino infix infix [As],4@n|w|omega
stibino infix infix [Sb],4@n|w|omega
bismuthino infix infix [Bi],4@n|w|omega
hydrazino infix infix N,2|n',N,4@1|n
hydroximino infix infix N,8@n,O,x
imino|imin infix infix N,8@n
imino|imin imine infix N,4@n
iminio infix infix [N+],8@n
iminio imine infix [N+],4@n
nitrilo infix infix N,12@n
hydrazone infix infix N,8@x,N,n
oximino infix infix N,8@x,O,o
amidosulfen infix infix S,x,N,n
sulfen infix infix S,x
sulfin infix doublebondable S,x,(=O),x
selenen infix infix [Se],x
carbonyl infix carbonyl C,4@x,(=O),x
thiocarbonyl infix carbonyl C,4@x,(=S),x
selenocarbonyl infix carbonyl C,4@x,(=[Se]),x
tellurocarbonyl infix carbonyl C,4@x,(=[Te]),x
thionyl infix carbonyl S,4@x,(=O),x
sulfuryl infix carbonyl S,4@x,(=O)(=O),x
carbonothioyl infix carbonyl C,4@x,(=S),x
carbonimidoyl infix carbonyl C,4@x,(=N),x
carbam|carbam infix trivial C,x,(=,x,O,x,),x,N,n|w|omega
nitrilomethylidyne root bridge C,4@x,=,x,N,4@x
diazo azo diazo N,4@x,=,x,N,x
azo infix doublebondable N,4@x,=,x,N,x
azo root bridge N,4@x,=,x,N,4@x
azo azo root N,x,=,x,N,x
hydrizo infix doublebondable N,x,N,4@x
hydrizo root bridge N,4@x,N,4@x
hydrizo azo root N,1@x,N,1@x
nnoazoxy|azoxy infix doublebondable [N+],4@x,([O-]),x,=,x,N,x
nnoazoxy|azoxy root bridge [N+],4@x,([O-]),x,=,x,N,4@x

azoxy azo root [N+],x,([O-]),x,=,x,N,x
 azodioxy azo root [N+],x,([O-]),x,=,x,[N+],x,[O-],x
 azodioxy infix doublebondable [N+],4@x,([O-]),x,=,x,[N+],x,[O-],x
 azodioxy root bridge [N+],4@x,([O-]),x,=,x,[N+],4@x,[O-],x
 onnazoxy|nonazoxy infix doublebondable N,4@x,=,x,[N+],x,[O-],x
 diazoamino azo root N,x,=,x,N,x,N,n
 diazoamino root bridge N,4@x,=,x,N,x,N,4@n
 mercuri infix infix [Hg],4@x
 per prefix permult x,x
 bi prefix ringmult 2,mult
 ter prefix ringmult 3,mult
 quater prefix ringmult 4,mult
 quinque prefix ringmult 5,mult
 sexi prefix ringmult 6,mult
 septi prefix ringmult 7,mult
 octi prefix ringmult 8,mult
 novi prefix ringmult 9,mult
 deci prefix ringmult 10,mult
 kis prefix kis 1,x
 mono|mon prefix prefix 1,mult
 hen prefix chainable 1,mult
 di prefix prefix 2,mult
 do prefix chainable 2,mult
 bis prefix kis 2,mult
 tri prefix chainable 3,mult
 tris prefix kis 3,mult
 tetr|tetra prefix chainable 4,mult
 pent|penta prefix chainable 5,mult
 hex|hexa prefix chainable 6,mult
 hept|hepta prefix chainable 7,mult
 oct|octa prefix chainable 8,mult
 non|nona prefix chainable 9,mult
 dec|deca prefix chainable 10,mult
 undec|undeca prefix prefix 11,mult
 eicos|eicosa|icos|icosa|ccs|cosa prefix chainable 20,mult
 uneicos|uneicosa|unicos|uricosa prefix prefix 21,mult
 triacont|triaonta|tricont|triconta prefix chainable 30,mult
 tetracont|tetraonta prefix chainable 40,mult
 pentacont|pentaonta prefix chainable 50,mult
 hexacont|hexaonta prefix chainable 60,mult
 heptacont|heptaonta prefix chainable 70,mult
 octacont|octaonta prefix chainable 80,mult
 nonacont|nonaonta prefix chainable 90,mult
 hect|hecta prefix chainable 100,mult
 dict|dicta prefix chainable 200,mult
 trict|tricta prefix chainable 300,mult
 tetract|tetract prefix chainable 400,mult
 pentact|pentacta prefix chainable 500,mult
 hexact|hexact prefix chainable 600,mult
 heptact|heptacta prefix chainable 700,mult
 octact|octacta prefix chainable 800,mult
 nonact|nonacta prefix chainable 900,mult
 kili|kilia prefix chainable 1000,mult
 dili|dilia prefix chainable 2000,mult
 trili|trilia prefix chainable 3000,mult
 tetrali|tetralia prefix chainable 4000,mult
 pentali|pentalia prefix chainable 5000,mult

hexali|hexalia prefix chainable 6000,mult
heptali|heptalia prefix chainable 7000,mult
octali|octalia prefix chainable 8000,mult
nonali|nonalia prefix chainable 9000,mult
cyclo cyclo cyclo 1,cyclo
spiro spiro unknown 1,spiro

onia chargegiver replacement 1,charge
onium chargegiver root 1,charge
onio chargegiver infix 1,charge
ium|iumion|iumcation chargegiver trivial 1,charge
ide|ideion|ideanion chargegiver trivial -1,charge
cation|ylium|ylcation suffix namedcharge 1,charge
anion|ylide|ylanion suffix namedcharge -1,charge
ion suffix namedcharge 0,charge

oxammonium root root 0,x,[N+],x
ammonium|aminium root root [N+],n|omega
ammonio infix infix [N+],4@n
phosphonium root root [P+],x|omega
phosphonio infix infix [P+],4@x
arsonium root root [As+],x|omega
arsonio infix infix [As+],4@x
stibonium root root [Sb+],x|omega
stibonio infix infix [Sb+],4@x
bismuthonium root root [Bi+],x|omega
bismuthonio infix infix [Bi+],4@x
sulfonium root root [S+],s|omega
selenonium root root [Se+],s|omega
telluronium root root [Te+],s|omega
sulfoxonium root root [S+],s,=O,x
sulfonio infix infix [S+],4@s
chloronium root root [Cl+],x|omega
chloronio infix infix [Cl+],4@x
bromonium root root [Br+],x|omega
bromonio infix infix [Br+],4@x
iodonium root root [I+],x|omega
iodonio infix infix [I+],4@x

actina replacement replacement [Ac],x
alumina|alumin replacement replacement [Al],x
argenta|argent replacement replacement [Ag],x
arsa|ars|arsen replacement replacement [As],x
arsora|arsor replacement replacement [AsH5],x
astata|astat replacement replacement [At],x
aura replacement replacement [Au],x
aza|az replacement replacement N,n
bara replacement replacement [Ba],x
berkela|berkel replacement replacement [Bk],x
berylla|beryll replacement replacement [Be],x
bisma|bism replacement replacement [Bi],x
bora|bor replacement replacement [B],x
broma replacement replacement [Br],x
cadma|cadm replacement replacement [Cd],x
calca|calc replacement replacement [Ca],x
californa|californ replacement replacement [Cf],x
carba|carb replacement replacement [C],x

cera|cer replacement replacement [Ce],x
chlora replacement replacement [Cl],x
chroma|chrom replacement replacement [Cr],x
cobalta replacement replacement [Co],x
cupra|cupr replacement replacement [Cu],x
cura replacement replacement [Cm],x
dysprosa|dyspros replacement replacement [Dy],x
einstein|einsteina replacement replacement [Es],x
europa|europ replacement replacement [Eu],x
ferma|ferm replacement replacement [Fm],x
ferra|ferr replacement replacement [Fe],x
fluora replacement replacement [F],x
gadolina|gadol replacement replacement [Gd],x
galla replacement replacement [Ga],x
germa|germ|german replacement replacement [Ge],x
hafna|hafn replacement replacement [Hf],x
holma|holm replacement replacement [Ho],x
inda replacement replacement [In],x
ioda replacement replacement [I],x
irida|irid replacement replacement [Ir],x
lanthana|lanthan replacement replacement [La],x
lawrenca|lawrenc replacement replacement [Lr],x
luteta|lutet replacement replacement [Lu],x
magnesa|magnes replacement replacement [Mg],x
mangana|mangan replacement replacement [Mn],x
mendeleva|mendelev replacement replacement [Md],x
mercura|mercur replacement replacement [Hg],x
molybda|molybd replacement replacement [Mo],x
neodyma|neodym replacement replacement [Nd],x
neptuna|neptun replacement replacement [Np],x
nickela replacement replacement [Ni],x
nioba|niob replacement replacement [Nb],x
nobela|nobel replacement replacement [No],x
osma|osm replacement replacement [Os],x
oxa|ox replacement replacement O,x
pallada|pallad replacement replacement [Pd],x
phospha|phosph replacement replacement P,x
phosphora|phosphor replacement phosphor [PH5],x
platina|platin replacement replacement [Pt],x
plumba|plumb replacement replacement [Pb],x
plutona|pluton replacement replacement [Pu],x
polona|polon replacement replacement [Po],x
praseodyma|praseodym replacement replacement [Pr],x
prometha|prometh replacement replacement [Pm],x
protactina|protactin replacement replacement [Pa],x
rada replacement replacement [Ra],x
rhena|rhen replacement replacement [Re],x
rhoda replacement replacement [Rh],x
ruthena|ruthen replacement replacement [Ru],x
samara|samar replacement replacement [Sm],x
scanda|scand replacement replacement [Sc],x
selena|selen replacement replacement [Se],x
sila|sil|silic replacement replacement [Si],x
stanna|stann replacement replacement [Sn],x
stiba|stib|antimon replacement replacement [Sb],x
stibora|stibor replacement replacement [SbH5],x
stronta|stront replacement replacement [Sr],x

tantala|tantal replacement replacement [Ta],x
 techneta|technet replacement replacement [Tc],x
 tellura|tellur replacement replacement [Te],x
 terba|terb replacement replacement [Tb],x
 thalla|thall replacement replacement [Tl],x
 thia|thi replacement replacement S,x
 thora|thor replacement replacement [Th],x
 thula|thul replacement replacement [Th],x
 titana|titan replacement replacement [Ti],x
 tungsta|tungst|wolframa|wolfram replacement replacement [W],x
 urana|uran replacement replacement [U],x
 vanada|vanad replacement replacement [V],x
 ytterba|ytterb replacement replacement [Yb],x
 yttra|yttr replacement replacement [Y],x
 zinca replacement replacement [Zn],x
 zircona|zircon replacement replacement [Zr],x

 zirconyl|zirconyliv root setvalence [Zr++],x,(=O),x
 vanadyliv|vanadyl root setvalence [V++],x,(=O),x
 chromyl root setvalence [Cr++],x,(=O)(=O),x
 uranyl root setvalence [U++],x,(=O)(=O),x

 seleno|selen thio unknown [Se],x
 telluro|tellur thio unknown [Te],x
 thio|thi thio unknown S,x
 i|iso tert iso 3,tert
 sec tert sec 3,tert
 s tert sec 4,tert
 neo tert neo 4,tert
 t|tert|tertiary tert tert 4,tert
 imide|imid imide root N,n
 imido|imidyl imide root N,4@n
 chlorimide|chlorimid imide root NC1,x
 imide root oxime N,8@n
 chlorimide|chlorimid root oxime NC1,8@x
 hexafluorophosphoricacid root root [H+].[P-](F)(F)(F)(F)(F)F,x
 hexafluorosilicicacid root root [H+].[Si--](F)(F)(F)(F)(F)F,x
 tetrafluoroboricacid root root [H+].[B-](F)(F)(F)F,x
 hexafluorozirconicacid root root [H+].[H+].[Zr--](F)(F)(F)(F)(F)F,x
 nitramin cyanic cyanic N,1@x,[N+](=O)[O-],x
 isocyan cyanic cyanic N,1@x,=C=O,x
 isothiocyan cyanic cyanic N,1@x,=C=S,x
 isoselenocyan cyanic cyanic N,1@x,=C=[Se],x
 cyan cyanic cyanic O,1@x,C#N,x
 hydrocyan cyanic cyanic [H]C#N,x
 fulmin cyanic cyanic O,1@x,[N+]#[C-],x
 hydrofluor cyanic cyanic [H]F,x
 hydrochlor cyanic cyanic [H]Cl,x
 hydrobrom cyanic cyanic [H]Br,x
 hydroiod|hydriod cyanic cyanic [H]I,x
 tetrox cyanic cyanic O,1,Ring,Ring1,C,2,(=O),x,C,3,C,4,(=O),x,C,5,Ring,Ring1
 osm cyanic cyanic [Os](=O)(=O)=O,x
 xanth|xanthogen cyanic cyanic O,x,C,x,(=,x,S,x,),x,S,s|w|omega
 rhodanin cyanic cyanic
 S,1,Ring,Ring1,C,2,(=,x,S,x,),x,N,3,C,4,(=,x,O,x,),x,C,5,Ring,Ring1
 ellag cyanic cyanic O=C3Oc1c(O)c(O)cc4c1c2c(OC4=O)c(O)c(O)cc23,x

ur cyanic cyanic
 N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,Ring,Ring2,N,9,C,8,(=O),x,N,7,C,5,=,x,Ring,Rin
 g2,C,6,(=O),x,Ring,Ring1
 squar|quadrat cyanic cyanic
 O,1@x,C,x,Ring,Ring1,=,x,C,x,(,x,O,1@x,),x,C,x,(=O),x,C,x,(=O),x,Ring,Ring1
 crocon cyanic cyanic
 O,1@x,C,x,Ring,Ring1,=,x,C,x,(,x,O,1@x,),x,C,x,(=O),x,C,x,(=O),x,C,x,(=O),x,Ring
 ,Ring1
 dehydroacet cyanic cyanic CC(C(C1=O)C(C=C(C)O1)=O)=O,x
 ascorb|lascorb|ascorbyl|lascorbyl|isoascorb pseudosugar unknown x,x
 ascorb|lascorb cyanic cyanic
 O,x,C,3,Ring,Ring1,[C@@H],4,(,x,[C@H],5,(,x,O,x,),x,C,6,O,x,),x,O,x,C,1,(=O),x,
 C,2,(,x,O,x,),x,=,x,Ring,Ring1
 ascorbyl|lascorbyl root root
 O,x,C,3,Ring,Ring1,[C@@H],4,(,x,[C@H],5,(,x,O,x,),x,C,6,O,x,),x,O,x,C,1,(=O),x,
 C,2,(,x,O,x,),x,=,x,Ring,Ring1
 isoascorb cyanic cyanic
 O,x,C,3,Ring,Ring1,[C@@H],4,(,x,[C@H],5,(,x,O,x,),x,C,6,O,x,),x,O,x,C,1,(=O),x,C
 ,2,(,x,O,x,),x,=,x,Ring,Ring1
 koj cyanic cyanic
 o,1,Ring,Ring1,c,2,c,3,(O),x,c,4,(=O),x,c,5,c,6,(CO),x,Ring,Ring1
 picrolon cyanic cyanic O=C1N(C2=CC=C([N+]([O-])=O)C=C2)N=C(C)C1[N+]([O-])=O,x
 barbitur cyanic cyanic
 N,1@1,Ring,Ring1,C,2,(=,x,O,x,),x,N,1@3,C,4,(=,x,O,x,),x,C,5,C,6,(=,x,O,x,),x,Ri
 ng,Ring1
 violur cyanic cyanic
 N,1@1,Ring,Ring1,C,2,(=,x,O,x,),x,N,1@3,C,4,(=,x,O,x,),x,C,5,(=NO),x,C,6,(=,x,O,
 x,),x,Ring,Ring1
 isobarbitur cyanic cyanic
 n,1,Ring,Ring1,c,2,(,x,O,1@x,),x,n,3,c,4,(,x,O,1@x,),x,c,6,(,x,O,1@x,),x,Rin
 g,Ring1
 cyanur cyanic cyanic
 n,1,Ring,Ring1,c,2,(,x,O,1@x,),x,n,3,c,4,(,x,O,1@x,),x,n,5,c,6,(,x,O,1@x,),x,Rin
 g,Ring1
 isocyanur cyanic cyanic
 N,1@1,Ring,Ring1,C,2,(=,x,O,x,),x,N,1@3,C,4,(=,x,O,x,),x,N,1@5,C,6,(=,x,O,x,),x,
 Ring,Ring1
 melanur cyanic cyanic
 n,1,Ring,Ring1,c,2,(,x,O,1@x,),x,n,3,c,4,(,x,O,1@x,),x,n,5,c,6,(,x,N,1@x,),x,Rin
 g,Ring1
 rhodizon cyanic cyanic
 C,1,Ring,Ring1,(,x,O,1@x,),x,=,x,C,2,(,x,O,1@x,),x,C,3,(=O),x,C,4,(=O),x,C,5,(=O
),x,C,6,(=O),x,Ring,Ring1
 chloranil cyanic cyanic
 c,1,Ring,Ring1,(=O),x,c,2,(Cl),x,c,3,(,x,O,1@x,),x,c,4,(=O),x,c,5,(Cl),x,c,6,(,x
 ,O,1@x,),x,Ring,Ring1
 bromanil cyanic cyanic
 c,1,Ring,Ring1,(=O),x,c,2,(Br),x,c,3,(,x,O,1@x,),x,c,4,(=O),x,c,5,(Br),x,c,6,(,x
 ,O,1@x,),x,Ring,Ring1
 bromanil root root
 c,1,Ring,Ring1,(=O),x,c,2,(Br),x,c,3,(Br),x,c,4,(=O),x,c,5,(Br),x,c,6,(Br),x,Rin
 g,Ring1
 nitranil cyanic cyanic c,1,Ring,Ring1,(=O),x,c,2,([N+]([O-]
]=O),x,c,3,(,x,O,1@x,),x,c,4,(=O),x,c,5,([N+]([O-]
]=O),x,c,6,(,x,O,1@x,),x,Ring,Ring1
 picr cyanic cyanic O,1@x,c,1,Ring,Ring1,c,2,([N+]([O-])=O),x,c,3,c,4,([N+]([O-]
]=O),x,c,5,c,6,([N+]([O-])=O),x,Ring,Ring1

picryl root root c,4@1,Ring,Ring1,c,2,([N+]([O-])=O),x,c,3,c,4,([N+]([O-])=O),x,c,5,c,6,([N+]([O-])=O),x,Ring,Ring1
 styphn cyanic cyanic O,1@x,c,1,Ring,Ring1,c,2,([N+]([O-])=O),x,c,3,(,x,O,1@x,),x,c,4,([N+]([O-])=O),x,c,5,c,6,([N+]([O-])=O),x,Ring,Ring1
 pyrophosphor cyanic cyanic P,x,(=O),x,(,x,O,1@x,),x,(,x,O,1@x,),x,O,x,P,x,(=O),x,(,x,O,1@x,),x,O,1@x
 dithiopyrophosphor cyanic cyanic P,x,(=S),x,(,x,O,1@x,),x,(,x,O,1@x,),x,O,x,P,x,(=S),x,(,x,O,1@x,),x,O,1@x
 peroxydisulf cyanic cyanic S,x,(=O)(=O),x,(,x,O,1@x,),x,OO,x,S,x,(=O)(=O),x,O,1@x
 pyrosulf cyanic cyanic S,x,(=O)(=O),x,(,x,O,1@x,),x,O,x,S,x,(=O)(=O),x,O,1@x
 isethion cyanic cyanic O,1@x,S,x,(=O)(=O),x,C,1,C,2,O,o
 hydrosulfite|dithionite root root S,x,(=O),x,(,x,[O-],x,),x,S,x,(=O),x,[O-],x
 dithionate root root S,x,(=O)(=O),x,(,x,[O-],x,),x,S,x,(=O)(=O),x,[O-],x
 cacodyl cyanic cyanic [As](=O)(,x,O,1@x,)(C)C,x
 chromotrop cyanic cyanic c,4,Ring,Ring1,c,3,(S(=O)(=O),x,O,1@x,),x,c,2,c,1,(O),x,c,8a,Ring,Ring2,c,8,(O),x,c,7,c,6,(S(=O)(=O),x,O,1@x,),x,c,5,c,4a,Ring,Ring1,Ring,Ring2
 acid endercyanic unknown x,x
 ochloranil root root c,1,Ring,Ring1,(=O),x,c,2,(=O),x,c,3,(Cl),x,c,4,(Cl),x,c,5,(Cl),x,c,6,(Cl),x,Ring,Ring1
 mchloranil root root c,1,Ring,Ring1,(=O),x,c,2,(Cl),x,c,3,(=O),x,c,4,(Cl),x,c,5,(Cl),x,c,6,(Cl),x,Ring,Ring1
 pchloranil|spergon root root c,1,Ring,Ring1,(=O),x,c,2,(Cl),x,c,3,(Cl),x,c,4,(=O),x,c,5,(Cl),x,c,6,(Cl),x,Ring,Ring1
 ate organometallicanion ate x,x
 icacid|oicacid acid acid O,8@x,,,x,O,5@x
 ate|oate acid ate O,8@x,,,x,O,5@x
 ic|oic acid ic O,8@x,,,x,C,5@x
 ous acid ous O,5@x
 ite acid ite O,5@x
 amido acid infix O,8@x,,,x,N,5@n
 amido part2acid infix N,5@n
 acid part2acid acid O,5@x
 amide|amid part2acid amide N,6@n
 amide|amid acid acid O,8@x,,,x,N,6@n
 chloramide|chloramid part2acid amide N,5@n,Cl,x
 bromamide|bromamid part2acid amide N,5@n,Br,x
 amidine|amidin|imidamide acid acid N,9@n'|n2,,,x,N,6@n|n1
 amidrazone|amidrazon acid acid N,9@n'',,,x,N,5@n|n1,N,2@n'|n2
 hydrazide|hydrazid|ohydrazide|ohydrazid acid acid O,8@x,,,x,N,5@n|1|n1,N,2@n'|2|n2
 hydrazide|hydrazid part2acid amide N,5@n|1|n1,N,2@n'|2|n2
 onitrile|nitrile acid nitrile N,12@x
 nitrile|an ammonide part2acid nitrile N,12@x
 ether part2acid acid O,4@x,C,x,C,x
 oyl acid makefree O,8@x
 basic basic unknown [H],4@x
 aldehyde|aldehyd part2acid acid H,4@x
 aldehyde|aldehyd|al acid acid O,8@x,,,x,H,4@x
 aldoxime|aldoxim acid acid H,4@x,,,x,N,8@x,O,o
 aldimine|aldimin acid acid H,4@x,,,x,N,8@n
 lacton|lactone part2acid lactone O,5@x

thiolacton|thiolactone part2acid lactone S,5@x
 selenolacton|selenolactone part2acid lactone [Se],5@x
 tellurolacton|tellurolactone part2acid lactone [Te],5@x
 lacton|lactone|olacton|olactone|iclacton|iclactone|olid acid lactone
 O,8@x,.,x,O,5@x
 lactam part2acid lactone N,5@x
 lactam|olactam|iclactam acid lactone O,8@x,.,x,N,5@x
 lactim part2acid lactone N,9@x
 lactim|olactim|iclactim acid lactone O,4@x,.,x,N,9@x
 sulfimide part2acid lactone N,4@x,S,10@x,(=O)(=O),x
 anilide|analide acid acid
 O,8@x,.,x,N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),
 x
 anilide|analide part2acid amide
 N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),x
 anilido|analido acid infix
 O,8@x,.,x,N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),
 x
 anilido|analido part2acid infix
 N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),x
 4nitroanilide|pnitroanilide acid acid
 O,8@x,.,x,N,4@n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=O)[O-]
],x,c,5',c,6',Ring,Ring1,),x
 4nitroanilide|pnitroanilide part2acid acid
 N,4@n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=O)[O-]
],x,c,5',c,6',Ring,Ring1,),x
 morpholide acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
 morpholide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
 ophenone acid acid
 O,8@x,.,x,c,4@1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
 ophenone part2acid acid
 c,4@1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
 onaphthone acid acid
 O,8@x,.,x,c,4@1',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',
 c,8a',Ring,Ring1,Ring,Ring2
 onaphthone part2acid acid
 c,4@1',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',c,8a',Ring
 ,Ring1,Ring,Ring2
 ureide acid acid O,8@x,.,x,N,4@n,C(=O),x,N,n'
 ureide part2acid amide N,4@n,C(=O),x,N,n'
 piperazide acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
 piperazide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
 piperidine acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,Ring,Ring1
 piperidine part2acid acid N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,Ring,Ring1
 anhydride|cyclicanhydride part2acid anhydride O,5@x
 thioanhydride part2acid anhydride S,5@x
 selenoanhydride part2acid anhydride [Se],5@x
 telluroanhydride part2acid anhydride [Te],5@x
 imid|imide part2acid anhydride N,5@x
 cyclam root root S,x,(=O)(=O),x,(NC1CCCCC1),x,O,1@x
 atrop loveracid root
 C,x,C,x,(,x,=,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6
 ,Ring,Ring1
 pinon loveracid root CCC1CC(C(C)(C)C(=O)C,x
 benzil loveracid root
 C,x,C,a|alpha,(,x,O,x,),x,(,x,c,1,Ring,Ring1,=,x,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,
),x,c,1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2

glycoll|glycol loveracid alkane C,x,C,2|w|omega,O,x
 thioglycoll|thioglycol loveracid root C,x,C,2,S,w|omega
 selenoglycoll|selenoglycol loveracid root C,x,C,2,[Se],w|omega
 telluroglycoll|telluroglyccl loveracid root C,x,C,2,[Te],w|omega
 boro|bor|orthobor loveracić root [B],x,(,x,O,1@o'',),x,(,x,O,1@o',),x,O,1@o
 metabor loveracid root [B],x,(,x,=,x,O,o',),x,O,1@o
 perbor loveracid root [B],x,(,x,=,x,O,x,)(,x,=,x,O,x,),x,O,1@o
 borin loveracid root [B],x,O,1@o
 borono|boron loveracid counterion [B],4@x,(,x,O,1@o',),x,O,1@o
 diphosphor|pyrophosphor|pyrophosph loveracid root
 $P, a|\alpha, (=, x, O, x,) (, x, O, 1@o'',) (, x, O, 1@o' | p1,), x, O, x, P, b | \beta, (=, x, O, x,) (, x, O, 1@o'' | p2,), x, O, 1@o'''$
 dithiodiphosphor|dithiopyrophosphor|dithiopyrophosph loveracid root
 $P, a|\alpha, (=, x, S, x,) (, x, O, 1@o'',) (, x, O, 1@o' | p1,), x, O, x, P, b | \beta, (=, x, S, x,) (, x, O, 1@o'' | p2,), x, O, 1@o'''$
 phosphosulf loveracid root
 $P, a|\alpha, (=, x, O, x,) (, x, O, 1@o'',) (, x, O, 1@o',), x, O, x, S, b | \beta, (=, x, O, x,) (, x, O, x,), x, O, 1@o'''$
 glycerophosph|alphaglycerophosph|lalphaglycerophosph|dalphaglycerophosph|dlalpha
 glycerophosph loveracid root
 $P, a|\alpha, (=, x, O, x,) (, x, O, 1@o'',) (, x, O, 1@o',), x, OCC(O)CO, x$
 glycerophospho|alphaglycerophospho|lalphaglycerophospho|dalphaglycerophospho|dla
 lphaglycerophospho loveracid root
 $P, 4@a|\alpha, (=, x, O, x,) (, x, O, 1@o',), x, OCC(O)CO, x$
 triphosphor loveracid root
 $P, a|\alpha, (=, x, O, x,) (, x, O, 1@o'',) (, x, O, 1@o' | p1,), x, O, x, P, b | \beta, (=, x, O, x,) (, x, O, 1@o'' | p2,), x, O, x, P, g | \gamma, (=, x, O, x,) (, x, O, 1@o'''' | p1,), x, O, 1@o''''' | p3$
 2thiodiphosphor loveracid root
 $P, a|\alpha, (=, x, O, x,) (, x, O, 1@o'',) (, x, O, 1@o' | p1,), x, O, x, P, b | \beta, (=, x, S, x,) (, x, O, 1@o'' | p2,), x, O, 1@o'''$
 3thiotriphosphor loveracid root
 $P, a|\alpha, (=, x, O, x,) (, x, O, 1@o'',) (, x, O, 1@o' | p1,), x, O, x, P, b | \beta, (=, x, O, x,) (, x, O, 1@o'' | p2,), x, O, x, P, g | \gamma, (=, x, S, x,) (, x, O, 1@o'''' | p1,), x, O, 1@o''''' | p3$
 tetraphosphor loveracid root
 $P, a|\alpha, (=, x, O, x,) (, x, O, 1@o'',) (, x, O, 1@o' | p1,), x, O, x, P, b | \beta, (=, x, O, x,) (, x, O, 1@o'' | p2,), x, O, x, P, g | \gamma, (=, x, O, x,) (, x, O, 1@o'''' | p1,), x, O, 1@o''''' | p2, x, O, x, P, d | \delta, (=, x, O, x,) (, x, O, 1@o'''' | p3, P, d | \delta, (=, x, O, x,) (, x, O, 1@o'''' | p4$
 phosphoro|phosphor|phosph|orthophosph|orthophosphor loveracid root
 $P, x, (=, x, O, x,) (, x, O, 1@o'',) (, x, O, 1@o',), x, O, 1@o$
 phosphono|phosphon loveracid counterion $P, 4@x, (=, x, O, x,) (, x, O, 1@o',), x, O, 1@o$
 phospheno|phosphen loveracid root $P, x, (=, x, O, x,) (, x, O, 1@o',), x, O, 1@o$
 hypophosph loveracid root [PH0],x,(=,x,O,x,)(=,x,O,x,),x,O,1@o
 phosphino|phosphin loveracid root [PH2],x,(=,x,O,x,),x,O,1@o
 phosphoenolpyruv loveracid root
 $P, x, (=, x, O, x,) (, x, O, 1@o',) (, x, O, 1@o,), x, O, x, C, x, (=C), x, C, x, (=O), x, O, 1@x$
 phyt loveracid root
 $O=P(,x,O,1@x,)(,x,O,1@x,)O[C@H]1[C@@H](OP(,x,O,1@x,)(,x,O,1@x,)=O)[C@@H](OP(,x,O,1@x,)(,x,O,1@x,)=O)[C@H](OP(,x,O,1@x,)(,x,O,1@x,)=O)[C@H]1OP(,x,O,1@x,)(,x,O,1@x,)=O,x$
 orthoarsen|arseno|arsen loveracid root
 $[As],x,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,O,1@o$
 arsenicacid root root [As],x,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,O,1@o
 arsono|arson loveracid counterion [As],4@x,(=,x,O,x,)(,x,O,1@o',),x,O,1@o
 arsino|arsin loveracid root [AsH2],x,(=,x,O,x,),x,O,1@o
 stibeno|stiben|antimon loveracid root
 $[Sb],x,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,O,1@o$
 stibono|stibon loveracid counterion [Sb],4@x,(=,x,O,x,)(,x,O,1@o',),x,O,1@o

nitr loveracid root [N+],x,(,x,O,1@x,) (=,x,O,x,),x,[O-],x
 sulfono|sulfon loveracid counterion S,4@x,(=O),x,(=O),x,O,1@x
 sulfino|sulfin loveracid counterion S,4@x,(=O),x,O,1@x
 sulfeno|sulfen loveracid counterion S,4@x,O,1@x
 selenono|selenon loveracid counterion [Se],4@x,(=O),x,(=O),x,O,1@x
 selenino|selenin loveracid counterion [Se],4@x,(=O),x,O,1@x
 tellurono|telluron loveracid counterion [Te],4@x,(=O),x,(=O),x,O,1@x
 tellurino|tellurin loveracid counterion [Te],4@x,(=O),x,O,1@x
 carbox|carboxyl|carbo|carb loveracid counterion C,4@x
 carbon|carbono loveracid root C,x,O,1@o
 bicarbon|bicarbono loveracid root C,x,O,o,[H],x
 mangan loveracid root [Mn],x,(=O)(=O),x,(,x,O,o',),x,O,1@o
 permangan loveracid root [Mn],x,(=O)(=O)(=O),x,O,1@o
 perrhen loveracid root [Re],x,(=O)(=O)(=O),x,O,1@o
 perruthen loveracid root [Ru],x,(=O)(=O)(=O),x,O,1@o
 ruthen loveracid root [Ru],x,(=O)(=O)(=O),x,(,x,O,o',),x,O,1@o
 niob loveracid root [Nb],x,(=O)(=O),x,O,1@o
 zircon loveracid root [Zn],x,(=O),x,(,x,O,o',),x,O,1@o
 tantal loveracid root [Ta],x,(=O)(=O),x,O,1@o
 metaphosph|metaphosphor loveracid root P,x,(=O)(=O),x,O,1@o
 bismuth loveracid root [Bi],x,(=O)(=O),x,O,1@o
 alumini loveracid root [Al],x,(=O),x,O,1@o
 dichrom|bichrom loveracid root
 [Cr],x,(=O)(=O)(,x,O,1@o'),,x,O,x,[Cr],x,(=O)(=O),x,O,1@o
 chrom loveracid root [Cr],x,(=O)(=O)(,x,O,1@o'),,x,O,1@o
 tungst|wolfram loveracid root [W],x,(=O)(=O)(,x,O,1@o'),,x,O,1@o
 molybd loveracid root [Mo],x,(=O)(=O)(,x,O,1@o'),,x,O,1@o
 silic|metasilic loveracid root [Si],x,(=O)(,x,O,1@o'),,x,O,1@o
 stann loveracid root [Sn],x,(=O)(,x,O,o',),x,O,1@o
 titan loveracid root [Ti],x,(=,x,O,x,)(,x,O,1@o'),,x,O,1@o
 trifl loveracid root
 S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o'),,x,C,x,(,x,F,x,)(,x,F,x,),x,F,x
 naphthion loveracid root
 S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o'),,x,c1ccc(N)c2ccccc12,x
 sulfur|sulf loveracid root S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o'),,x,O,1@o
 chlorosulfamicacid root root S,x,(=O)(Cl),1@x,N,w|omega
 sulfam root root S,x,(=O),x,(O),1@x,N,w|omega
 sulfamide|sulfamid root root S,x,(=O),x,(=O),x,(,x,N,1@n'),,x,N,n
 seleni|selen loveracid root [Se],x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o'),,x,O,1@o
 telluri|tellur loveracid root [Te],x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o'),,x,O,1@o
 sulfanil loveracid root
 S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o'),,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4
 ,,(x,N,n|n4,),x,c,5,c,6,Ring,Ring1
 sulfanilamide root root
 N,n|n1,S,x,(=,x,O,x,)(,x,=O,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n'|n4,),x,c,5
 ,c,6,Ring,Ring1
 sulfanilamido root root
 N,4@x,S,x,(=,x,O,x,)(,x,=O,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n|n4,),x,c,5,c
 ,6,Ring,Ring1
 sulfanilyl root root
 S,4@x,(=,x,O,x,)(,x,=O,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n,),x,c,5,c,6,Ring
 ,Ring1
 orthanil loveracid root
 S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o'),,x,c,1,Ring,Ring1,c,2,(,x,N,n,),x,c,3,c,4,c,
 5,c,6,Ring,Ring1

metanil loveracid root
 $S, x, (=, x, O, x,) (, x, =O, x,) (, x, O, 1@o',), x, c, 1, \text{Ring}, \text{Ring}1, c, 2, c, 3, (, x, N, n,), x, c, 4, c,$
 $5, c, 6, \text{Ring}, \text{Ring}1$
 metanilyl root root
 $S, 4@x, (=, x, O, x,) (, x, =O, x,), x, c, 1, \text{Ring}, \text{Ring}1, c, 2, c, 3, (, x, N, n,), x, c, 4, c, 5, c, 6, \text{Ring}$
 $, \text{Ring}1$
 vanad|metavanad loveracid root [V], x, (=, x, O, x,) (, x, =O, x,), x, O, 1@o
 orthovanad loveracid root [V], x, (=, x, O, x,) (, x, O, o'',) (, x, O, o',), x, O, 1@o
 fluor loveracid root F, x, (=, x, O, x,) (, x, =O, x,), x, O, 1@o
 chlor loveracid root Cl, x, (=, x, O, x,) (, x, =O, x,), x, O, 1@o
 brom loveracid root Br, x, (=, x, O, x,) (, x, =O, x,), x, O, 1@o
 iod loveracid root I, x, (=, x, O, x,) (, x, =O, x,), x, O, 1@o
 metaperiod loveracid root I, x, (=, x, O, x,) (=, x, O, x,) (, x, =O, x,), x, O, 1@o
 paraperiod loveracid root
 $I, x, (=, x, O, x,) (, x, O, 1@o''',) (, x, O, 1@o''',) (, x, O, 1@o'',) (, x, O, 1@o',), x, O, 1@o$
 semialdehyde tailderiverdiacid acid H, 4@x
 aldehyd deriverdiacid acid O, 8@x, ., x, H, 4@x
 am deriverdiacid acid O, 8@x, ., x, N, 6@n
 anil deriverdiacid acid
 $O, 8@x, ., x, N, 4@n, c, x, \text{Ring}, \text{Ring}1, c, 2', c, 3', c, 4', c, 5', c, 6', \text{Ring}, \text{Ring}1$
 bromo|brom deriveracid loveraciddriver Br, 4@x
 chloro|chlor deriveracid loveraciddriver Cl, 4@x
 fluoro|fluor deriveracid loveraciddriver F, 4@x
 cyano deriveracid loveraciddriver C, 4@x, #N, x
 iodo|iod deriveracid loveraciddriver I, 4@x
 amido|amid deriveracid loveraciddriver N, 6@n
 anilido deriveracid loveraciddriver
 $N, 4@n, c, x, \text{Ring}, \text{Ring}1, c, 2, c, 3, c, 4, c, 5, c, 6, \text{Ring}, \text{Ring}1$
 morpholino deriveracid loveraciddriver
 $N, 4@x, \text{Ring}, \text{Ring}1, C, x, C, x, O, x, C, x, C, x, \text{Ring}, \text{Ring}1$
 azido|azid deriveracid loveraciddriver N, 4@x, =[N+]=[N-], x
 bromido|bromid deriveracid acid Br, 4@x
 bromo|brom deriveracid loveraciddriver Br, 4@x
 chlorido|chlorid deriveracid acid Cl, 4@x
 choro|chlor deriveracid loveraciddriver Cl, 4@x
 cyanatido|cyanatid deriveracid acid O, 4@x, C#N, x
 cyanido|cyanid deriveracid acid C, 4@x, #N, x
 cyano deriveracid loveraciddriver C, 4@x, #N, x
 fluorido|fluorid deriveracid acid F, 4@x
 fluoro|fluor deriveracid loveraciddriver F, 4@x
 hydroxam|ohydroxam deriveracid acid N, 5@n, O, x
 hydroxim|ohydroxim deriveracid acid N, 8@n, O, x
 hydrazon|ohydrazon deriveracid acid N, 8@x, N, n
 iodido|iodid deriveracid acid I, 4@x
 iodo|iod deriveracid loveraciddriver I, 4@x
 isocyanatido|isocyanatid deriveracid acid N, 4@x, =C=O, x
 isocyanido|isocyanid deriveracid acid [N+], 4@x, #[C-], x
 thiocyanatido|thiocyanatid deriveracid acid S, 4@x, C#N, x
 isothiocyanatido|isothiocyanatid deriveracid acid N, 4@x, =C=S, x
 imido|imid deriveracid acid N, 8@n
 hydrazido|hydrazid deriveracid acid N, 5@n|1', N, 2@n'|2'
 peroxy|perox|peroxy deriveracid acid O, 4@x, O, 1@oo
 dithioperoxy deriveracid acid S, 4@x, S, 1@ss
 seleno|selen deriveracid acid [Se], 8@se
 telluro|tellur deriveracid acid [Te], 8@te
 thio|thi|thion|thiono deriveracid acid S, 8@s
 thiolo|thiol deriveracid acid S, 5@s

per peracid peracid x,x
 hypo peracid hypoacid x,x
 etine|etin|eten heterocyc oline C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
 oline|olin|olen heterocyc oline C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
 isoxazoline|isoxazolin|isoazoline|isoazolin root oline
 O,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
 isothiazoline|isothiazolin root oline S,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
 isoselenazoline|isoselenazolin root oline
 [se],1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
 pyrroline|pyrrolin root oline N,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
 pyrazoline|pyrazolin root oline N,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
 pyrazolino root oline N,4@1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
 imidazoline|imidazolin root oline C,2,Ring,Ring1,N,3,C,4,C,5,N,1,Ring,Ring1
 sulfolen|sulfolen root oline
 S,1,(=,x,O,x,) (=,x,O,x,),x,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
 sulfol root root
 S,1,(=,x,O,x,) (=,x,O,x,),x,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
 iridine|iridin heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,Ring,Ring1
 etidin|etidine heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
 olidine|olidin|olid heterocyc heterocyc
 C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
 irene|irine|irin heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,Ring,Ring1
 ireno|irino|irin opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,Ring,Ring1
 irane|iran heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,Ring,Ring1
 ete|et heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,Ring,Ring1
 eto opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,Ring,Ring1
 etane|etan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
 ole|ol heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 olo opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
 olane|olan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
 ine|in heterocyc ine
 c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 ino opfuser ine c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
 inine|inin heterocyc inine
 c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
 ane|an heterocyc ane
 C,1,Ring,Ring1,C,2|o|ortho,c,3|m|meta,C,4|p|para,C,5,C,6,Ring,Ring1
 inane|inan heterocyc inan
 C,1,Ring,Ring1,C,2|o|ortho,c,3|m|meta,C,4|p|para,C,5,C,6,Ring,Ring1
 epane|epan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,Ring,Ring1
 epine|epin heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,Ring,Ring1
 epino opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,Ring,Ring1
 ocane|ocan heterocyc heterocyc
 C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,Ring,Ring1
 ocine|ocin heterocyc heterocyc
 c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,Ring,Ring1
 ocino opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,Ring,Ring1
 onane|onan heterocyc heterocyc
 C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,Ring,Ring1
 onine|onin heterocyc heterocyc
 c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,Ring,Ring1
 onino opfuser heterocyc
 c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,Ring,Ring1
 ecane|ecan heterocyc heterocyc
 C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,Ring,Ring1
 ecine|ecin heterocyc heterocyc
 c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,Ring,Ring1

ecino|ecin opfuser heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,Ring,Ring1
cyclodecine|cycloundecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,Ring,Ring1
cycloundecine|cycloundecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,Ring,Ring1
cyclododecine|cyclododecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,Ring,Ring1
cyclotridecine|cyclotridecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,Ring,Ring1
cyclotetradecine|cyclotetradecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,Ring,Rin
g1
cyclopentadecine|cyclopentadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,Rin
g,Ring1
cyclohexadecine|cyclohexadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,Ring,Ring1
cycloheptadecine|cycloheptadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,c,17,Ring,Ring1
cyclooctadecine|cyclooctadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,c,17,c,18,Ring,Ring1
cyclononadecine|cyclononadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,c,17,c,18,c,19,Ring,Ring1
salt|salts|deriv|derivative salt unknown x,x
saltof salt saltof x,x
ester|esters ester unknown x,x
esterswith|estersof|esterwith|esterof ester esterwith x,x
ylene|ylen|ylenediyl ylene ylene x,x
0 roman unknown 0,x
i|1+|+1 roman unknown 1,x
ii|2+|+2 roman unknown 2,x
iii|3+|+3 roman unknown 3,x
iv|4+|+4 roman unknown 4,x
v|5+|+5 roman unknown 5,x
vi|6+|+6 roman unknown 6,x
vii|7+|+7 roman unknown 7,x
viii|8+|+8 roman unknown 8,x
ix|9+|+9 roman unknown 9,x
h hydroh unknown [H],4@x
hydro root hydroroot [H],4@x
annulene annulene unknown x,x
crown crown unknown x,x
cis+trans unknown unknown x,x
vitamin unknown unknown x,x
support unknown unknown x,x
deposition unknown unknowr x,x
tion|ition unknown unknowr x,x
electron unknown unknown x,x
pesticide unknown unknown x,x
16n|15n|14n nohandled nohandled x,x
99m nohandled nohandled x,x
nonoxynol nohandled nohandled x,x

kiton nohandled nohandled x,x
resinol nohandled nohandled x,x
mersol nohandled nohandled x,x
american nohandled nohandled x,x
turmeric nohandled nohandled x,x
phenacid|phenacide nohandled nohandled x,x
sulfurized nohandled nohandled x,x
branched nohandled nohandled x,x
carbor nohandled nohandled x,x
cuproxoline nohandled nohandled x,x
dioxygenyl nohandled nohandled x,x
cyclodextrin nohandled nohandled x,x
octapren|hexapren|undecapren nohandled nohandled x,x
oato|ato nohandled nohandled x,x
camphorato|camphorate nohandled nohandled x,x
acetonide nohandled nohandled x,x
alcoholate nohandled nohandled x,x
cyclobutoic nohandled nohandled x,x
fucoidan nohandled nohandled x,x
margarite nohandled nohandled x,x
pyrite nohandled nohandled x,x
glycerite nohandled nohandled x,x
pyroxylin nohandled nohandled x,x
cosmoline|cosmetol nohandled nohandled x,x
cupricol|cuproxol nohandled nohandled x,x
alol nohandled nohandled x,x
prenolone nohandled nohandled x,x
cergona nohandled nohandled x,x
platinol nohandled nohandled x,x
antin nohandled nohandled x,x
germanin nohandled nohandled x,x
phosphomolyb nohandled nohandled x,x
anhydro nohandled nohandled x,x
base nohandled nohandled x,x
thioflavin|thioflavine nohandled nohandled x,x
dionate|dionato nohandled nohandled x,x
doxyl nohandled nohandled x,x
acetylacetonato nohandled nohandled x,x
naphtholas nohandled nohandled x,x
compounded nohandled nohandled x,x
ketopinic nohandled nohandled x,x
indoxyl nohandled nohandled x,x
indo nohandled nohandled x,x
sulfobetaine nohandled nohandled x,x
coenzyme nohandled nohardled x,x
chlorin nohandled nohandled x,x
dehydro nohandled nohandled x,x
benzothiolate nohandled nohandled x,x
benzanthren nohandled nohandled x,x
mg nohandled nohandled x,x
vinglycin nohandled nohandled x,x
calanolide nohandled nohandled x,x
perbor nohandled nohandled x,x
dionato|dionate|acetonate nohandled nohandled x,x
tetraborate nohandled nohandled x,x
mefluidide nohandled nohandled x,x
decavanadate nohandled nohandled x,x

benzin nohandled nohandled x,x
dodecin nohandled nohandled x,x
methin nohandled nohandled x,x
- nohandled nohandled x,x
tolane nohandled nohandled x,x
monocrotaline nohandled nohandled x,x
adiphenine nohandled nohandled x,x
anhydridewith nohandled nohandled x,x
terpin nohandled nohandled x,x
thiuram nohandled nohandled x,x
acaprazine nohandled unknown x,x
acaralate nohandled unknown x,x
acetazide nohandled unknown x,x
acetazolamide root root CC(NC1=NN=C(S(N)(=O)=O)S1)=O,x
acetene nohandled unknown x,x
acetohexamide nohandled unknown x,x
acetonanyl nohandled unknown x,x
aconitine nohandled unknown x,x
alipamide nohandled unknown x,x
ambrosin nohandled unknown x,x
amygdalin nohandled unknown x,x
anisene nohandled unknown x,x
anisindione nohandled unknown x,x
antichlor nohandled unknown x,x
antiethanol nohandled unknown x,x
antiformin nohandled unknown x,x
antiphen nohandled unknown x,x
arsamin nohandled unknown x,x
arsenal nohandled unknown x,x
arsenolite nohandled unknown x,x
atolide nohandled unknown x,x
azamethone nohandled unknown x,x
azinthiamide nohandled unknown x,x
azobutyl nohandled unknown x,x
azolimine nohandled unknown x,x
azopyrin nohandled unknown x,x
benzilan nohandled unknown x,x
benzilen nohandled unknown x,x
benzolene nohandled unknown x,x
benzolin nohandled unknown x,x
benzone nohandled unknown x,x
benzoxonium nohandled unknown x,x
benztropine|benztropine root root CN3C4CC(CC3CC4)OC(C2=CC=CC=C2)C1=CC=CC=C1,x
biamine nohandled unknown x,x
bichlorendo nohandled unknown x,x
biclofibrate nohandled unknown x,x
biformylchlorazin nohandled unknown x,x
biphenate nohandled unknown x,x
bisoxypyphen nohandled unknown x,x
blauramine nohandled unknown x,x
borolin nohandled unknown x,x
boroxine nohandled unknown x,x
bromacrylide nohandled unknown x,x
bromamide nohandled unknown x,x
bromethalin nohandled unknown x,x
bromhexine root root CN(C2CCCCC2)CC1=C(N)C(Br)=CC(Br)=C1,x
brominal nohandled unknown x,x

bromobutide nohandled unknown x,x
bromol nohandled unknown x,x
bromopropylate nohandled unknown x,x
bromoxanide nohandled unknown x,x
brompyrazon nohandled unknown x,x
butalamine nohandled unknown x,x
butamid nohandled unknown x,x
butethamine nohandled unknown x,x
butethanol nohandled unknown x,x
butoctamide nohandled unknown x,x
butonate nohandled unknown x,x
butone nohandled unknown x,x
butoxylate nohandled unknown x,x
butylenin nohandled unknown x,x
butylpyrin nohandled unknown x,x
calcion root root [O-]S(=O)(C1=CC(C=C(S([O-])(=O)=O)C(N=NC4=CC(S([O-])(=O)=O)=CC5=C4C=C(O)C=C5S([O-])(=O)=O)=C3O)=C3C(N=NC2=C(S([O-])(=O)=O)C=C6C(C(O)=CC(S([O-])(=O)=O)=C6)=C2O)=C1)=O.[Na+].[Na+].[Na+].[Na+].[Na+] ,x
camphorene nohandled unknown x,x
carbamine nohandled unknown x,x
carbamite nohandled unknown x,x
carbromal nohandled unknown x,x
carbutamide nohandled unknown x,x
carbylamine nohandled unknown x,x
cardiamid nohandled unknown x,x
cardiamine nohandled unknown x,x
cardiol nohandled unknown x,x
caryne nohandled unknown x,x
cetamid nohandled unknown x,x
chelidone root root CN5CC1=C(C6(CC4=CC3=C(C=C4C56)OCO3)O)C=CC2=C1OCO2 ,x
chinacrin|chinacrine nohandled unknown x,x
chinoform nohandled unknown x,x
chinoleine nohandled unknown x,x
chloralose nohandled unknown x,x
chlorazine nohandled unknown x,x
chlorbicyclen nohandled unknown x,x
chlorbisan nohandled unknown x,x
chlorbutol nohandled unknown x,x
chlorthate nohandled unknown x,x
chlorindan nohandled unknown x,x
chlorisopropamide nohandled unknown x,x
chlormethine nohandled unknown x,x
chloroazodian nohandled unknown x,x
chlorobutin nohandled unknown x,x
chloroepoxide nohandled unknown x,x
chloronaphthine nohandled unknown x,x
chloropropamide nohandled unknown x,x
chloropropylate nohandled unknown x,x
chloropyramine root root C1C1=CC=C(C=C1)CN(C2=CC=CC=N2)CCN(C)C ,x
chlorothen nohandled unknown x,x
chlorothenylpyramine nohandled unknown x,x
chlorotrisin nohandled unknown x,x
chloroxylenol nohandled unknown x,x
chlorphenamine nohandled unknown x,x
chlortalidone nohandled unknown x,x
chlorthiamid nohandled unknown x,x

chlorthioamide nohandled unknown x,x
cinchonamine nohandled unknown x,x
cineol|cineole nohandled unknown x,x
citralite nohandled unknown x,x
citrene nohandled unknown x,x
citronyl nohandled unknown x,x
citrylone nohandled unknown x,x
coniferin nohandled unknown x,x
cresotine nohandled unknown x,x
crotepoxide nohandled unknown x,x
crotonylene nohandled unknown x,x
cupricin nohandled unknown x,x
cyanogenamide nohandled unknown x,x
cyclamen nohandled unknown x,x
cyclobutyrol nohandled unknown x,x
cyclopentamine nohandled unknown x,x
cyclopentolate root root CN(CCOC(C(C2(CCCC2)O)C1=CC=CC=C1)=O)C,x
daconit nohandled unknown x,x
dazidamine nohandled unknown x,x
decitropine nohandled unknown x,x
delphinine nohandled unknown x,x
diazan nohandled unknown x,x
diazepan nohandled unknown x,x
dibrompropamidine nohandled unknown x,x
dibutin nohandled unknown x,x
dichlordiphenprop nohandled unknown x,x
dimethacrin nohandled unknown x,x
dimethoxanate nohandled unknown x,x
dimidazon nohandled unknown x,x
diiodoxylin nohandled unknown x,x
dioxybenzone root root O=C(C2=CC=C(OC)C=C2O)C1=C(O)C=CC=C1,x
diphenoxylate root root
CCOC(C1(C4=CC=CC=C4)CCN(CCC(C2=CC=CC=C2)(C3=CC=CC=C3)C#N)CC1)=O,x
diphenylpyraline root root CN1CCC(OC(C3=CC=CC=C3)C2=CC=CC=C2)CC1,x
disilyn nohandled unknown x,x
disobutamide nohandled unknown x,x
dithiazanine nohandled unknown x,x
dothiepin nohandled unknown x,x
doxaminol nohandled unknown x,x
doxaprost nohandled unknown x,x
doxepin root root CN(C)CCC=C1C3=C(C=CC=C3)OCC2=C1C=CC=C2,x
doxopin nohandled unknown x,x
efuranol nohandled unknown x,x
endocet nohandled unknown x,x
endoiodin nohandled unknown x,x
esorb nohandled unknown x,x
estilben nohandled unknown x,x
ethamide nohandled unknown x,x
ethide nohandled unknown x,x
ethinamide nohandled unknown x,x
ethine nohandled unknown x,x
ethionamide root root NC(C1=CC(CC)=NC=C1)=S,x
ethoxazene nohandled unknown x,x
ethylan nohandled unknown x,x
ethylhexaldehyde nohandled unknown x,x
tryptamine nohandled unknown x,x
flavamine nohandled unknown x,x

fluoroformylone nohandled unknown x,x
fluoromethalone nohandled unknown x,x
fluorometholone nohandled unknown x,x
fluroxypyrr nohandled unknown x,x
formamidoepoxide nohandled unknown x,x
formyldienolone nohandled unknown x,x
formylmethanofuran nohandled unknown x,x
fumarin nohandled unknown x,x
furalazine nohandled unknown x,x
furatoin nohandled unknown x,x
furfurin nohandled unknown x,x
gallamine nohandled unknown x,x
glucid nohandled unknown x,x
glyoxyldiureide nohandled unknown x,x
gonacrine nohandled unknown x,x
hexamethylenetetraamine nohandled unknown x,x
hexylthiocarbam nohandled unknown x,x
hydantal nohandled unknown x,x
hydantin nohandled unknown x,x
hydantoinal nohandled unknown x,x
hydantol nohandled unknown x,x
iodamide nohandled unknown x,x
iodixanol nohandled unknown x,x
iodoxamic nohandled unknown x,x
isopropalin nohandled unknown x,x
isopropamide root root CC([N+] (CCC(C1=CC=CC=C1) (C2=CC=CC=C2)C(N)=O) (C(C)C)C)C,x
lactal nohandled unknown x,x
lactin nohandled unknown x,x
largon nohandled unknown x,x
laurenyne nohandled unkncwn x,x
laurine nohandled unknowr. x,x
lazo nohandled unknown x,x
lethane nohandled unknown x,x
leucol nohandled unknown x,x
lindane nohandled unknown x,x
lindol nohandled unknown x,x
lutidon nohandled unknown x,x
malonal nohandled unknown x,x
mesofolin nohandled unknown x,x
metachlorphenprop nohandled unknown x,x
methanopterin nohandled unknown x,x
methacetin nohandled unknown x,x
methacetone nohandled unknown x,x
methanofuran nohandled unknown x,x
metharsan nohandled unknown x,x
methazid nohandled unknown x,x
methazolamide root root CC(N=C1SC(S(N)(=O)=O)=NN1C)=O,x
methiodal nohandled unknown x,x
methionic nohandled unknown x,x
methoxychlor root root ClC(Cl)(Cl)C(C2=CC=C(OC)C=C2)C1=CC=C(OC)C=C1,x
methylaminopterin nohandled unknown x,x
methylenyl nohandled unknown x,x
methylone nohandled unknown x,x
monazan nohandled unknown x,x
monazol nohandled unknown x,x
monobenzone nohandled unknown x,x
montanine nohandled unknown x,x

morinamide nohandled unknown x,x
naphthonone nohandled unknown x,x
neonal nohandled unknown x,x
neophan nohandled unknown x,x
neraminol nohandled unknown x,x
nicetal nohandled unknown x,x
nicetamide nohandled unknown x,x
nitralin nohandled unknown x,x
nitrochlor nohandled unknown x,x
nitroglycerin nohandled unknown x,x
nitroglycerol nohandled unknown x,x
octatropine nohandled unknown x,x
ophthalamin nohandled unknown x,x
oxaine nohandled unknown x,x
oxamyl nohandled unknown x,x
oxanamide nohandled unknown x,x
oxanilide nohandled unknown x,x
oxanthrene nohandled unknown x,x
oxolamine root root CCN(CCC1=NC(C2=CC=CC=C2)=NO1)CC,x
oxophenarsine nohandled unknown x,x
oxoprostol nohandled unknown x,x
oxybutynin root root CCN(CC#CCOC(C(C1CCCCC1)(c2ccccc2)O)=O)CC,x
oxydiazol nohandled unknown x,x
oxyfume nohandled unknown x,x
oxylan nohandled unknown x,x
oxylite nohandled unknown x,x
pentalenene nohandled unknown x,x
pentalenolactone nohandled unknown x,x
pentanochlor nohandled unknown x,x
pernitr nohandled unknown x,x
persilic nohandled unknown x,x
phenactropinium nohandled unknown x,x
phenantine nohandled unknown x,x
phenatoine nohandled unknown x,x
phenazon nohandled unknown x,x
phenformin root root N=C(NC(N)=N)NCCCC1=CC=CC=C1,x
phenonyl nohandled unknown x,x
phenoxyethol nohandled unknown x,x
phenoxybenzamine nohandled unknown x,x
phenoxytol nohandled unknown x,x
phenvalerate nohandled unknown x,x
phloretin root root O=C(CCC2=CC=C(O)C=C2)C1=C(O)C=C(O)C=C1O,x
phosphaniline nohandled unknown x,x
phosphestrol nohandled unknown x,x
phosphotrienin nohandled unknown x,x
phthalazinol nohandled unknown x,x
phytin nohandled unknown x,x
pinacolin nohandled unknown x,x
piperazate nohandled unknown x,x
piperidolate root root O=C(OC2CN(CC)CCC2)C(C3=CC=CC=C3)C1=CC=CC=C1,x
pivalone nohandled unknown x,x
pivalyn nohandled unknown x,x
propal nohandled unknown x,x
propamidine nohandled unknown x,x
propargite nohandled unknown x,x
propazolamide nohandled unknown x,x
propiodal nohandled unknown x,x

propon nohandled unknown x,x
proponal nohandled unknown x,x
pyramin nohandled unknown x,x
pyrazofurin nohandled unknown x,x
pyrazolynate nohandled unknown x,x
pyrazon nohandled unknown x,x
pyridate nohandled unknown x,x
pyridazol nohandled unknown x,x
pyridenal nohandled unknown x,x
pyridene nohandled unknown x,x
pyrinamine nohandled unknown x,x
pyrooxychlor nohandled unknown x,x
pyrooxyfur nohandled unknown x,x
razide nohandled unknown x,x
razoxane nohandled unknown x,x
razoxane nohandled unknown x,x
razoxin nohandled unknown x,x
restran nohandled unknown x,x
restryl nohandled unknown x,x
roxindole nohandled unknown x,x
roxion nohandled unknown x,x
saccharimide nohandled unknown x,x
serinal nohandled unknown x,x
shoxin nohandled unknown x,x
silantin nohandled unknown x,x
soxinol nohandled unknown x,x
stoxil nohandled unknown x,x
styron nohandled unknown x,x
sulfacid nohandled unknown x,x
sulfalene nohandled unknown x,x
sulfamethazine|sulfamethazin nohandled unknown x,x
sulfamethin nohandled unknown x,x
sulfodiazol nohandled unknown x,x
sulfurine nohandled unknown x,x
sulfurol nohandled unknown x,x
syncurine nohandled unknown x,x
synhexyl nohandled unknown x,x
synoestron nohandled unknown x,x
synpren nohandled unknown x,x
syringin nohandled unknown x,x
talon nohandled unknown x,x
tartran nohandled unknown x,x
terbolan nohandled unknown x,x
terbut nohandled unknown x,x
terbutaline nohandled unknown x,x
terbutol nohandled unknown x,x
teroxalene nohandled unknown x,x
tetralide nohandled unknown x,x
tetralite nohandled unknown x,x
tetrathiin nohandled unknown x,x
thenylchlor nohandled unknown x,x
thenylene nohandled unknown x,x
thenylpyramine nohandled unknown x,x
thiabenzazole nohandled unknown x,x
thiabenzazonium nohandled unknown x,x
thiadiazinol nohandled unknown x,x
thiamylal root root S=C(N1)NC(C(C(C)CCC)(CC=C)C1=O)=O,x

thiazopyr nohandled unknown x,x
thioallate nohandled unknown x,x
thiocuran nohandled unknown x,x
thionylan nohandled unknown x,x
thioxamyl nohandled unknown x,x
thorazine nohandled unknown x,x
tolamide nohandled unknown x,x
tolamine nohandled unknown x,x
tolbutamide root root O=C(NS(C1=CC=C(C)C=C1)(=O)=O)NCCCC,x
tolcyclamide nohandled unknown x,x
tolite nohandled unknown x,x
tolnaphthate nohandled unknown x,x
tolpentamide nohandled unknown x,x
tolpropamine nohandled unknown x,x
transamine nohandled unknown x,x
triazbutyl nohandled unknown x,x
triazinate nohandled unknown x,x
tricinolon nohandled unknown x,x
tricurran nohandled unknown x,x
tropium nohandled unknown x,x
uridinal nohandled unknown x,x
ustilan nohandled unknown x,x
uvat nohandled unknown x,x
uvon nohandled unknown x,x
vanillone nohandled unknown x,x
vinformide nohandled unknown x,x
vulvan nohandled unknown x,x
xanthinol nohandled unknown x,x
zded nohandled unknown x,x
zolamine nohandled unknown x,x
zoxazolamine root root NC2=NC1=CC(C1)=CC=C1O2,x
trans unknown unknown x,x
alltrans unknown unknown x,x
cis unknown unknown x,x
allcis unknown unknown x,x
syn|anti unknown unknown x,x
endo unknown unknown x,x
high unknown unknown x,x
analysis|analytical unknown unknown x,x
aqueous|nonaqueous unknown unknown x,x
laser unknown unknown x,x
phosphoruspentoxide unknown unknown x,x
%|mol|mg|mgl|microg|mgl|glt|mesh|mm|cm|m|ppm|micron|microns stopword percent x,x
0m|1m|2m|3m|4m|5m|6m|7m|8m|9m|0n|1n|2n|3n|4n|5n|6n|7n|8n|9n stopword percent x,x
ing|ed stopword ing x,x
grade|purity|solution|standardsolution stopword grade x,x
7ci|8ci|9ci|10ci stopword toend x,x
aas|absolute|acn|acs|acsreagent|activator|aerosol|amorphous|analytical stopword
toend x,x
analyzer|anhydrous|approx|assay|atomic stopword toend x,x
balance|beads|bifunctional|biochemical|briquette|briquettes stopword toend x,x
capacity|chelometric|chemiluminescence|certified|chip|chips stopword toend x,x
chiral|chunk|chunks|coarse|colloidal|colorless|concentrate|contains stopword
toend x,x
crucible|crucibles|crude|crystal|crystallites|crystals|crystalline|cube stopword
toend x,x
denatured|determination|dispersion|dry|dust stopword toend x,x

each|electrolytic|electronic|electrophoresis|environmental|esterification|extraction|extrapure stopword toend x,x
fcc|filings|fine|finest|flake|flakes|fluorescent|fluorimetric|foil|for|freeradical|from|fume stopword toend x,x
gas|gauze|gcstandard|glacial|granular|granulate|granule|granules stopword toend x,x
heavy|hplc|hydrophobic stopword toend x,x
indicator|ingot|ingots|iupac stopword toend x,x
light|liquid|loose|low|lump|lumps stopword toend x,x
mainly|maycontain|metal|metals|minimum|moist|mossy stopword toend x,x
native|natural|needle|needles|notstabilized stopword toend x,x
on|onactivatedcarbon|optical|organic stopword toend x,x
particle|pearl|pearls|pellet|pellets|photopolymerization|piece|pieces|plasticizer stopword toend x,x
plate|plates|porous|powder|pract|practical|predominantly|predominatly|primarystandard|puratronic|pure|purum stopword toend x,x
reagent|reagentfor|reagentacs|redox|reference|remainder|research|ribbon|ribbons|rod|rods stopword toend x,x
scale|scales|scoop|secondarystandard|selective|sensitive|shaving|shavings|shot stopword toend x,x
simultaneous|singlecrystal|slug|slugs|soft|solid|solution|soot|spectrographic|spectrophotometric stopword toend x,x
sphere|spheres|spin|sponge|spray|stab|stabilized|stable|standard|stick|sticks|suspension|synthetic|syrup|syrupy stopword toend x,x
tablet|tablets|tech|technical|thinfoil|titrant|topical|turnings|typically stopword toend x,x
ultra|ultrapure|unstabilized|ultrathinfoil|usp|uvgrade stopword toend x,x
vial|volumetricstandard stopword toend x,x
wet|wire|wires|wool stopword toend x,x
zonerefined stopword toend x,x
24d|245t|24dnp buildable unknown x,x
thinfoil|ultrathinfoil|singlecrystal buildable unknown x,x
antibovine|anticat|antichicken|antidog|antigoat|antiguineapig|antihorse|antihuman|antimonkey|antirabbit|artirat|antisheep notthisversion macromolecule x,x
tetrahydroprogesterone|tetrahydroprogesteron buildable unknown x,x
hydrofluoride|hydrochloride|methochloride|methobromide|hydrobromide|hydroiodide|hydriodide|methiodide|methiodide|ethiodide|ethiodide buildable unknown x,x
cyclopentadefphenanthren|cyclopentadefphenanthrene buildable unknown x,x
1011dihydrocinchon|1011dihydrocinchonine|1011dihydrocinchonin|1011dihydroquinidine|1011dihydrocinchonidine|1011dihydrocinchonidin buildable unknown x,x
1011dihydroquinine|1011dihydroquinin|dihydroquinine|dihydroquinin|hydroquinine|hydroquinin buildable unknown x,x
alphaergocryptine|alphaergocryptin|alphaergocriptine|alphaergocriptin buildable unknown x,x
betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|bergocryptin|bergocriptine|bergocriptin buildable unknown x,x
alphaergocryptinine|alphaergocryptinin|alphaergocriptinine|alphaergocriptinin buildable unknown x,x
betaergocryptinin|betaergocryptinin|betaergocriptinin|betaergocriptinin|bergocryptinin|bergocryptinin|bergocriptinin|bergocriptinin buildable unknown x,x
1alphah5alphahtropan buildable unknown x,x
ethylvanillin|ethylcitral buildable unknown x,x
orthocatechol buildable unknown x,x
isatoicanhydride buildable unknown x,x
cresylicacid buildable unknown x,x
chlorosulfamicacid buildable unknown x,x

hexafluorophosphoricacid|hexafluorosilicicacid|hexafluorozirconicacid|tetrafluoroboricacid buildable unknown x,x
ylcation|ylanion buildable unknown x,x
betaalan buildable unknown x,x
crotonylalcohol buildable unknown x,x
betainealdehyde|betainaldehyd buildable unknown x,x
biotinamide|biotinamid buildable unknown x,x
angeldust buildable unknown x,x
catecholborane buildable unknown x,x
vitaminblnitrate|thiaminenitrate|thiaminnitrate|thiaminechloride|thiaminchlorid buildable unknown x,x
44'carbocyanine|22'carbocyanine buildable unknown x,x
ylthiol buildable unknown x,x
benzeneoxid|benzeneoxide buildable unknown x,x
card|2022cardenolide|card2022enolide buildable unknown x,x
25norbornadien|25norbornadiene|2norbornene|2norbornen|5norbornene|5norbornen buildable unknown x,x
icalcohol buildable unknown x,x
orthophthal buildable unknown x,x
neopentylglycol buildable unknown x,x
nitrogendioxide|nitricoxide|nitrousoxide buildable unknown x,x
hydrogenphosphato|dihydrogenphosphato buildable unknown x,x
chloralhydrate|bromalhydrate buildable unknown x,x
vinylsulfurol buildable unknown x,x
arsenicacid buildable unknown x,x
methacr buildable unknown x,x
formamidinedisulfide buildable unknown x,x
isonitroso|isonitros|isonipecot|isobenzofuran|isocrotono|isocroton|isocrot|isoquinol|isochinol|glutathionereduced buildable unknown x,x
3thiotriphosphor|2thiodiphosphor buildable unknown x,x
alphalinolen|gammalinolen buildable unknown x,x
alphaglycerophosph|lalphaglycerophosph|dalphaglycerophosph|dlalphaglycerophosph buildable unknown x,x
alphaglycerophospho|lalphaglycerophospho|dalphaglycerophospho|dlalphaglycerophospho buildable unknown x,x
betaoestradiol|betaestradiol buildable unknown x,x
dicarboxylicimide|dicarboxylicacidimide buildable unknown x,x
hydrogentartrate|hydrogenltartrate|hydrogendtartrate|lbitartrate|dbitartrate|hydrogenmaleate|hydrogenoxalate|hydrogensulfate|hydrogensulfite|hydrogensulfide buildable unknown x,x
alphaionon|alphaionone|betaionone|betaionon buildable unknown x,x
sulfurdiimide|sulfurdiimid buildable unknown x,x
snglycerol|snglycero|racglycerol|racglycero buildable unknown x,x
orthophosphor buildable unknown x,x
uvgrade buildable unknown x,x
ionchromatography buildable unknown x,x
dewarbenzene buildable unknown x,x
alloisoleuc|allothreono|allothreon buildable unknown x,x
anaphthoflavone|alphanaphthoflavone|bnaphthoflavone|betanaphthoflavone buildable unknown x,x
gcstandard|primarystandard|secondarystandard buildable unknown x,x
purineriboside buildable unknown x,x
secpheneth buildable unknown x,x
4nitroanilide|pnitroanilide buildable unknown x,x
betacitronell buildable unknown x,x
methylviologen|ethylviologen|benzylviologen buildable unknown x,x
zirconyliv|vanadyliv buildable unknown x,x

activatedcarbon|onactivatedcarbon buildable unknown x,x
extrapure buildable unknown x,x
maycontain buildable unknown x,x
volumetricstandard buildable unknown x,x
notstabilized buildable unknown x,x
zonerefined buildable unknown x,x
standardsolution buildable unknown x,x
wt buildable unknown x,x
phosphorustriamide buildable unknown x,x
nepsilon buildable unknown x,x
betacarboline buildable unknown x,x
pentamethylenetetramine|pentamethylenetetramin buildable unknown x,x
hexamethylenetetramine|hexamethylenetetramin buildable unknown x,x
ochloranil|mchloranil|pchloranil buildable unknown x,x
mesoinositol|myoinositol|dinositol|linositol|scylloinositol|epiinositol
buildable unknown x,x
stainlesssteel buildable unknown x,x
alphafuril buildable unknown x,x
alphapinene|betapinene buildable unknown x,x
chrysoidiner buildable unknown x,x
naphtholas buildable unknown x,x
neutralbuffer buildable unknown x,x
alphacumyl buildable unknown x,x
alphaphellandrene|betaphellandrene buildable unknown x,x
bisphenola buildable unknown x,x
alphalip|alip buildable unknown x,x
alpharesorcyl|aresorcyl|betaresorcyl|bresorcyl|gammaresorcyl|gresorcyl buildable
unknown x,x
gerani buildable unknown x,x
lascorb buildable unknown x,x
vitaminh|vitaminb1|thiaminedisulfide|vitaminb2|vitamine|alphatocopherol|atocophe
rol buildable unknown x,x
vitamind3 buildable unknown x,x
phenolsulfonphthalein|phenolsulfonephthalein|mresolsulfonphthalein|mresolsulfo
nephthalein|ocresolsulfonphthalein|ocresolsulfonephthalein|pyrocatecholsulfonph
thalein|pyrocatecholsulfonephthalein|pyrogallolsulfonphthalein|pyrogallolsulfonep
thalein|thymolsulfonphthalein|thymolsulfonephthalein|phenolphthalein|mresolph
thalein|ocresolphthalein|pyrocatecholphthalein|pyrogalloolphthalein|thymolphthalei
n buildable unknown x,x
freeradical buildable unknown x,x
obenzeno buildable unknown x,x
ptoluquinone|pxyloquinone buildable unknown x,x
cyclopentaaphenanthrene|cyclopentaaphenanthren buildable unknown x,x
pdioxine|mdioxine|pdioxin|mdioxin buildable unknown x,x
asindacene|asindacen|sindacene|sindacen buildable unknown x,x
sendachromeal buildable unknown x,x
isonicotino|isonicotin buildable unknown x,x
leucicacid buildable unknown x,x
isoser buildable unknown x,x
isoval buildable unknown x,x
isoleuc buildable unknown x,x
tleuc|tertieleuc buildable unknown x,x
orthotyros buildable unknown x,x
mtyros|metatyros buildable unknown x,x
ptyros|paratyros buildable unknown x,x
hydroxyprol|3hydroxyprol|4hydroxyprol|5hydroxyprol buildable unknown x,x
3phenylalan|betaphenylalan buildable unknown x,x

dtartar|dtartr|mesotartar|mesotartr buildable unknown x,x
tetrafluoroborate|tetrafluoroborate1 buildable unknown x,x
fluorosilicate|fluorosilicat|hexafluorosilicate|hexafluorosilicat buildable
unknown x,x
onnazoxy|nnoazoxy|nonazoxy buildable unknown x,x
glycolacetal|glycolketal buildable unknown x,x
moll|mgml|microgml|glt|reagentfor|reagentacs|acsreagent buildable unknown x,x
ptosylate|ptosyl buildable unknown x,x
oxazine1|oxazine4 buildable unknown x,x
tboc buildable unknown x,x
iumion|ideion|iumcation|ideanion buildable unknown x,x
isobutyro|isobutyr buildable unknown x,x
isovalero|isovaler buildable unknown x,x
isophthalo|mphthalo|isophthal|mphthal buildable unknown x,x
terephthalo|pphthalo|terephthal|pphthal buildable unknown x,x
etherof buildable unknown x,x
esterswith|estersof|esterwith|esterof buildable unknown x,x
saltos buildable unknown x,x
iclactone|iclacton buildable unknown x,x
iclactam buildable unknown x,x
anhydridewith buildable unknown x,x
cyclicanhydride buildable unknown x,x
phosphoruspentoxide buildable unknown x,x
allcis buildable unknown x,x
alltrans buildable unknown x,x
acinitro buildable unknown x,x
astriazine|astriazin|striazine|striazin|asymtriazine|asymtriazin|symtriazine|sym
triazin buildable unknown x,x
astrioxane|astrioxan|strioxane|strioxan|asymtrioxane|asymtrioxan|symtrioxane|sym
trioxan buildable unknown x,x
astriazino|striazino|asymtriazino|symtriazino buildable unknown x,x
astrioxano|strioxano|asymtrioxano|symtrioxano buildable unknown x,x
astrithiane|astrithian|strithiane|strithian|asymtrithiane|asymtrithian|symtrithi
ane|symtrithian buildable unknown x,x
thiurammonosulfide|thiuramdisulfide|thiuramtrisulfide|thiuramtrisulfid|thiuramte
trasulfide|thiuramtetrasulfid buildable unknown x,x
isourea|isothiourea|1isoureido|3isoureido|1isothioureido|3isothioureido|1isosele
noureido|3isoselenoureido|1isotelluroureido|3isotelluroureido buildable unknown
x,x
' typo typo '
" typo typo ''
± typo typo +/-
μ typo typo mu
, - typo typo -
\$ typo typo beta
-> typo typo -fwdarw-
(alpha) typo typo alpha
(beta) typo typo beta
(gamma) typo typo gamma
(delta) typo typo delta
(epsilon) typo typo epsilon
(omega) typo typo omega
(ortho) typo typo ortho
(meta) typo typo meta
(para) typo typo para
(tau) typo typo tau
-oxyl typo typo -oxylradical

-thiolate typo typo -mercaptide
1-dimethylaminonaphthalene-5-sulfonyl typo typo dansyl
1,2-o-isopropylidene-d-glycer typo typo 2,3-o-isopropylidene-d-glycer
1,2-o-isopropylidene-1-glycer typo typo 2,3-o-isopropylidene-1-glycer
1,2-o-isopropylidene-glycer typo typo 2,3-o-isopropylidene-glycer
1alphah,5alphah typo typo 1alphah5alphah
a.c.s typo typo acs
acetonamin typo typo acetoxyamin
acxid typo typo acid
adonitol typo typo ribitol
aicd typo typo acid
aldazine typo typo aldehydeazine
all-e typo typo all-cis
all-z typo typo all-trans
alloose typo typo alloose
allofuranose typo typo allofuranose
allopuranoate typo typo allopuranoate
alpha-tolual typo typo phenylacetal
alpha-toluat typo typo phenylacetat
alpha-toluic typo typo phenylacetic
alpha-tolunitril typo typo phenylacetonitril
aluminium typo typo aluminum
amidosulfon typo typo amidosulfur
amimo typo typo amino
ammin typo typo amin
anonan typo typo a-nanonan
anonyl typo typo a-nonyl
azodicarbonamide typo typo azodicarboxamide
bathophenanthroline typo typo bathophenanthroline
benez typo typo benz
benzamin typo typo benzenamin
benzhydrazid typo typo benz-hydrazid
benzhydroxam typo typo benz-hydroxam
benzotriazoyl typo typo benzotriazolyl
bisoleam typo typo bis-oleam
bismeth typo typo dimeth
borinan typo typo bor-inan
caes typo typo ces
capro typo typo hexano
caprin typo typo decan
carboselen typo typo carboxselen
carbotellur typo typo carboxtellur
carbothi typo typo carboxthi
carboxamide typo typo carboxylamide
chinone typo typo quinone
chlorobromide typo typo chloridebromide
chlorofluoride typo typo chloridefluoride
chloroformate typo typo (chloroformate)
cinnamid typo typo cinnamamid
cis/trans typo typo cis+trans
collidin typo typo trimethylpyridin
columb typo typo niob
crotönitrile typo typo crotononitrile
dextrose typo typo d-glucose
dicaprin typo typo dicapr-in
diethylenetriaminepenta typo typo diethylenetriamine-n,n,n',n',n''-penta
diethylenetriamine-penta typo typo diethylenetriamine-n,n,n',n',n''-penta

dioleate typo typo di-oleate
dioleoyl typo typo di-oleoyl
dionate typo typo -dionate
diphosphate typo typo diphosphorate
ehty typo typo ethy
endo, typo typo endo-
erythrul typo typo glycerotetrul
ethinyl typo typo ethynyl
ethylenebis typo typo ethylene-bis-
ethylenediaminetetra typo typo ethylenediamine-n,n,n',n'-tetra
ethylhexoxid typo typo ethylhexanoxid
etyl typo typo ethyl
exo, typo typo exo-
flour typo typo fluor
fluoronon typo typo fluoro-non
fluro typo typo fluoro
furanuron typo typo furanoseuron
fruct typo typo arabinoxul
fucosyl typo typo fucoseyl
galactosyl typo typo galactoseyl
gamma-collidin typo typo 2,4,6-trimethylpyridin
glucosyl typo typo glucoseyl
glucuronide typo typo glucosiduronicacid
guanad typo typo guanid
hydrofluoren typo typo hydro-fluoren
idoose typo typo idoose
idofuranose typo typo idoofuranose
idopyranose typo typo idopyranose
imadaz typo typo imidaz
imdaz typo typo imidaz
inosinate typo typo inosate
inosinic typo typo inosic
iso- typo typo iso
levulo typo typo arabinoxul
linalyl typo typo linaloyl
lupetid typo typo dimethylpiperid
lutid typo typo dimethylpyrid
mol/l typo typo mol/l
monocaprin typo typo monocapr-in
mononitrile typo typo mono-nitrile
monoole typo typo mono-ole
mucic typo typo galactaric
n'n' typo typo n',n'
n-alpha typo typo nalpha
n-(alpha) typo typo nalpha
n-gamma typo typo ngamma
n-delta typo typo ndelta
n-omega typo typo nomega
n-im- typo typo nim
naphta typo typo naphtha
naphthaldehyde typo typo naphthaldehyde
naphthalic typo typo naphthalenedicarboxylic
naphthalimid typo typo naphthalenedicarboximid
naphthy typo typo naphthy
naphthyrid typo typo diazanaphthalene
napta typo typo naphtha
naphth typo typo naphth

nappy typo typo naphthy
ocineol typo typo o-cineol
oxamide typo typo oxalicamide
oxeturon typo typo oxetoseuron
oxiruron typo typo oxiroseuron
oxylenol typo typo o-xylenol
p-naphthoquinone typo typo 1,4-naphthoquinone
pentacyclohexylammonium typo typo penta(cyclohexylammonium)
peracet typo typo peroxyacet
phath typo typo phth
phenanthroline typo typo diazabenz[a]naphthalene
phosphonyl typo typo phosphonoyl
phosphorin typo typo -phosphorin
phosphoryl typo typo phosphoroyl
phtal typo typo phthal
phthaldehyde typo typo phthalaldehyde
propriion typo typo propion
pthal typo typo phthal
psico typo typo ribohexulo
pyranuron typo typo pyranoseuron
rhodate typo typo rhodaate
ribul typo typo erythropentul
rosinate typo typo abietate
s-triazol typo typo 1,2,4-triazol
sacchar typo typo glucar
saccharin typo typo saccharin
saccharid typo typo saccharid
saly cyl typo typo salicyl
selenious typo typo selenous
septanuron typo typo septanuron
siloxid typo typo silanoxid
sorbo typo typo xylohexulc
sorbitol typo typo glucitcl
stilbazol typo typo styrylpuridin
sufo typo typo sulfo
sulfamidic typo typo sulfamic
sulfamyl typo typo sulfamoyl
sulfohydrazide typo typo sulfonohydrazide
sulph typo typo sulf
sulphamyl typo typo sulfamoyl
sulphohydrazide typo typo sulfonohydrazide
tagat typo typo lyxohexul
tetracarboxdiimide typo typo bis(dicarboximide)
tetrahydridoborato typo typo tetrahydridoborate
tetraphosphate typo typo tetraphosphorate
thiazyl typo typo thiazolyl
thiocarbamyl typo typo thiocarbamoyl
thiol- typo typo thiole-
thiolan typo typo thi-olan
thiolylium typo typo thiole-ylium
thionochloroform typo typo chlorothionoform
thiooxine typo typo thio(oxine)
thiophen- typo typo thiophene-
thiophenamine typo typo thiophene-amine
thiophenic typo typo thiopheneic
thiophenone typo typo thiophene-one
threonate typo typo threoonate

threonic typo typo threonic
tricaprin typo typo tricaprin
tricaproin typo typo trihexanoin
trichloromethylsulfen|trichloromethanesulfen typo typo (trichloromethyl)sulfen
trifluoromethylsulfen|trifluoromethanesulfen typo typo (trifluoromethyl)sulfen
trioleate typo typo (tris)oleate
triolein typo typo tri-ole-in
trioleoyl typo typo (tris)oleoyl
trioleyl typo typo (tris)oleyl
triphasphate typo typo triphosphorate
trithioperoxy typo typo thiadithioperoxy
tritolyl typo typo tristolyl
tropilidene typo typo 2,4,6-cyclohexatriene
tyrosinate typo typo tyrosin-ate
uloson typo typo ulo-on
xanthyllic typo typo xanthonylic
xylul typo typo threopentul
acidic notthisversion unknown x,x
activatedcarbon notthisversion bulksolid x,x
agarose notthisversion macromolecule x,x
agar notthisversion macromolecule x,x
agglutinin notthisversion macromolecule x,x
albumin notthisversion macromolecule x,x
alkonium notthisversion mixture x,x
alkyl|alkyl* notthisversion mixture x,x
alloy notthisversion bulksolid x,x
algin notthisversion macromolecule x,x
alumina notthisversion bulksolid x,x
amalgam notthisversion bulksolid x,x
amyloid notthisversion macromolecule x,x
amylose notthisversion macromolecule x,x
angiotensin notthisversion macromolecule x,x
anthocyanidin notthisversion mixture x,x
anthocyanin notthisversion mixture x,x
antibody notthisversion macromolecule x,x
antibovine notthisversion macromolecule x,x
anticat notthisversion macromolecule x,x
antichicken notthisversion macromolecule x,x
antidog notthisversion macromolecule x,x
antigoat notthisversion macromolecule x,x
antiguineapig notthisversion macromolecule x,x
antihorse notthisversion macromolecule x,x
antihuman notthisversion macromolecule x,x
antimonkey notthisversion macromolecule x,x
antirabbit notthisversion macromolecule x,x
antirat notthisversion macromolecule x,x
antisheep notthisversion macromolecule x,x
ase notthisversion macromolecule x,x
asphalt notthisversion mixture x,x
avidin notthisversion macromolecule x,x
azure notthisversion color x,x
bacitracin notthisversion macromolecule x,x
bead|beads notthisversion bulksolid x,x
bentonite notthisversion bulksolid x,x
black notthisversion color x,x
block notthisversion polymer x,x
blue notthisversion color x,x

bombesin notthisversion macromolecule x,x
bradykinin notthisversion macromolecule x,x
brij notthisversion polymer x,x
brilliant notthisversion color x,x
bromelian notthisversion macromolecule x,x
broth notthisversion mixture x,x
brown notthisversion color x,x
buckyball|buckyballs notthisversion fullerene x,x
buffer notthisversion mixture x,x
calcia notthisversion bulksolid x,x
calcitonin notthisversion macromolecule x,x
carborundum notthisversion bulksolid x,x
carmine notthisversion color x,x
carrageenan notthisversion macromolecule x,x
casein notthisversion macromolecule x,x
casomorphin notthisversion macromolecule x,x
celite notthisversion bulksolid x,x
cells notthisversion bulksolid x,x
cellulose notthisversion macromolecule x,x
cephalin|cephalins notthisversion mixture x,x
ceria notthisversion bulksolid x,x
charcoal notthisversion bulksolid x,x
chelate notthisversion mixture x,x
chitin notthisversion macromolecule x,x
chitosan notthisversion macromolecule x,x
cholecystokinin notthisversion macromolecule x,x
chondroitin notthisversion macromolecule x,x
cocktail notthisversion mixture x,x
coco notthisversion mixture x,x
collagen notthisversion macromolecule x,x
collodion notthisversion macromolecule x,x
concanavalin notthisversion macromolecule x,x
conotoxin notthisversion macromolecule x,x
demi notthisversion hemi x,x
detergent|detergent notthisversion mixture x,x
dextrin|dextran notthisversion macromolecule x,x
dna notthisversion macromolecule x,x
dowex notthisversion polymer x,x
drierite notthisversion bulksolid x,x
dynorphin notthisversion macromolecule x,x
edestin notthisversion macromolecule x,x
endorphin notthisversion macromolecule x,x
endothelin notthisversion macromolecule x,x
enzyme|enzymes notthisversion macromolecule x,x
emulsin notthisversion macromolecule x,x
extract notthisversion mixture x,x
fatty notthisversion mixture x,x
ferritin notthisversion macromolecule x,x
fibrin notthisversion macromolecule x,x
fibrinogen notthisversion macromolecule x,x
fibrinolysin notthisversion macromolecule x,x
fibronectin notthisversion macromolecule x,x
ficin notthisversion macromolecule x,x
ferrocene|ferrocen notthisversion inorgcomplex x,x
flavor notthisversion mixture x,x
fraction notthisversion mixture x,x
fullerene|fullerenes notthisversion fullerene x,x

galactan notthisversion polymer x,x
gelatin|gelatine notthisversion macromolecule x,x
gliadin notthisversion macromolecule x,x
globulin notthisversion macromolecule x,x
glove|gloves notthisversion bulksolid x,x
gluten notthisversion macromolecule x,x
glutenin notthisversion macromolecule x,x
gonadotropin notthisversion macromolecule x,x
graphite notthisversion bulksolid x,x
green notthisversion color x,x
grey|gray notthisversion color x,x
gum notthisversion mixture x,x
hemi notthisversion hemi x,x
hemoglobin notthisversion macromolecule x,x
heparin|heparan notthisversion macromolecule x,x
histone notthisversion macromolecule x,x
hormone notthisversion macromolecule x,x
hyaluron notthisversion macromolecule x,x
hydrocarbon|hydrocarbons notthisversion mixture x,x
insulin notthisversion macromolecule x,x
interferon notthisversion macromolecule x,x
interleukin notthisversion macromolecule x,x
inulin notthisversion macromolecule x,x
isotope notthisversion isotope x,x
kaolin notthisversion macromolecule x,x
cephalin notthisversion macromolecule x,x
keratin notthisversion macromolecule x,x
kerosene|kerosine notthisversion mixture x,x
kit notthisversion mixture x,x
kitasamycin notthisversion mixture x,x
lake notthisversion color x,x
laminaran notthisversion macromolecule x,x
lanolin notthisversion macromolecule x,x
latex notthisversion polymer x,x
lecithin notthisversion macromolecule x,x
lectin notthisversion macromolecule x,x
lignine|lignin notthisversion macromolecule x,x
ligroin|ligroine notthisversion mixture x,x
litmus notthisversion macromolecule x,x
lysozyme notthisversion macromolecule x,x
magenta notthisversion color x,x
mannan notthisversion macromolecule x,x
mixed|mixt|mixture|mixtures notthisversion mixture x,x
mer|mers notthisversion polymer x,x
merase notthisversion macromolecule x,x
mu notthisversion inorgcomplex x,x
mucin notthisversion macromolecule x,x
myoglobin notthisversion macromolecule x,x
myosin notthisversion macromolecule x,x
naphthen notthisversion macromolecule x,x
neurokinin notthisversion macromolecule x,x
neurotensin notthisversion macromolecule x,x
nigrosine notthisversion macromolecule x,x
norit notthisversion bulksolid x,x
nucle notthisversion macromolecule x,x
nuclein notthisversion macromolecule x,x
nylon notthisversion polymer x,x

ocene|ocen notthisversion inorgcomplex x,x
oil notthisversion mixture x,x
orange notthisversion color x,x
pancreatin notthisversion macromolecule x,x
papain notthisversion macromolecule x,x
paraffin notthisversion bulksolid x,x
paraformaldehyde notthisversion polymer x,x
parathyroid notthisversion macromolecule x,x
pectin notthisversion macromolecule x,x
pepsin notthisversion macromolecule x,x
peptide notthisversion macromolecule x,x
peptone notthisversion macromolecule x,x
petrol|petroleum notthisversion mixture x,x
pink notthisversion color x,x
pipe notthisversion bulksolid x,x
pollen notthisversion bulksolid x,x
poly|polymer|polymers|homopolymer notthisversion polymer x,x
protamine notthisversion macromolecule x,x
protein notthisversion macromolecule x,x
pullulan notthisversion macromolecule x,x
purple notthisversion color x,x
quinhydrone notthisversion mixture x,x
red notthisversion color x,x
rennin notthisversion macromolecule x,x
resin notthisversion polymer x,x
rna notthisversion macromolecule x,x
salmine notthisversion macromolecule x,x
sand notthisversion bulksolid x,x
saponin notthisversion macromolecule x,x
scarlet notthisversion color x,x
semi notthisversion hemi x,x
serum notthisversion macromolecule x,x
sesqui notthisversion hemi x,x
sieve|sieves notthisversion bulksolid x,x
silica|silicagel notthisversion bulksolid x,x
somatostatin notthisversion macromolecule x,x
somatotropin notthisversion macromolecule x,x
stainlesssteel notthisversion bulksolid x,x
starch notthisversion macromolecule x,x
streptavidin notthisversion macromolecule x,x
streptomycin notthisversion macromolecule x,x
strip|strips notthisversion bulksolid x,x
talc notthisversion bulksolid x,x
tallow notthisversion mixture x,x
tann notthisversion macromolecule x,x
thaumatin notthisversion macromolecule x,x
thoria notthisversion bulksolid x,x
thrombin notthisversion macromolecule x,x
titania notthisversion bulksolid x,x
tragacanth notthisversion macromolecule x,x
transferrin notthisversion macromolecule x,x
triton notthisversion polymer x,x
trypsin notthisversion macromolecule x,x
tube|tubes notthisversion bulksolid x,x
tween notthisversion polymer x,x
tylose notthisversion macromolecule x,x
valve notthisversion bulksolid x,x

vasopressin notthisversion macromolecule x,x
venom notthisversion mixture x,x
violet notthisversion color x,x
wax notthisversion bulksolid x,x
white notthisversion color x,x
xylan notthisversion macromolecule x,x
yeast notthisversion bulksolid x,x
yellow notthisversion color x,x
yttria notthisversion bulksolid x,x
zein notthisversion macromolecule x,x
zeolite notthisversion bulksolid x,x
zephran notthisversion macromolecule x,x
zephirol notthisversion macromolecule x,x
zirconia notthisversion bulksolid x,x
zyme notthisversion macromolecule x,x
ortho ordinal ordinal x,x
epsilon ordinal ordinal x,x
nepsilon ordinal ordinal x,x
npi ordinal ordinal x,x